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Supporting Information

Versatile Access to Nitrogen-Rich π-Extended Indolocarbazoles via a Pictet-Spengler Approach

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1 Experimental Procedures

1.1 General Information

Chemicals were bought from commercial suppliers (abcr, Acros, Alfa Aesar, Carbolution, Chempur, Fluka, Merck, Sigma Aldrich and TCI) and used as delivered. Anhydrous solvents were dispensed from a solvent purification system MB SPS-800. Solvents were degassed by freeze-pump-thaw technique. Deuterated solvents were bought from Eurisotop and Sigma Aldrich.

Melting points (mp) were measured in open glass capillaries on a Stuart SMP10 melting point apparatus and are uncorrected.

R_f-values were determined by analytical thin layer chromatography (TLC) on aluminum sheets coated with silica gel produced by Macherey-Nagel (ALUGRAM® Xtra SIL G/25 UV_{254}). Detection was accomplished using UV-light (254 and 365 nm) or a TLC staining solution (vanillin and ninhydrine).

Nuclear magnetic resonance (NMR) spectra were, if not mentioned otherwise, recorded at room temperature at the organic chemistry department of Heidelberg University under the supervision of Dr. J. Graf on the following spectrometers: Bruker Avance III 300 (300 MHz), Bruker Avance DRX 300 (300 MHz), Bruker Fourier 300 (300 MHz), Bruker Avance III 400 (400 MHz), Bruker Avance III 500 (500 MHz), Bruker Avance III 600 (600 MHz), Bruker Avance NEO 700 (700 MHz). $CDCl_3$ was filtered through a plug of aluminum oxide to remove acid impurities. Chemical shifts (δ) are given in ppm and coupling constants *J* in Hz. Spectra were referenced to residual solvent protons according to Fulmer *et al.*[1] or for TCE-d_2 to 6.00 ppm for ^{1}H and 73.8 ppm for ^{13}C. The following abbreviations were used to describe the observed multiplicities: for ^{1}H NMR spectra: s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sext =sextet, sept = septet, m = multiplet, dd = doublet of doublets, td = triplet of doublets, dt = doublet of triplets, br = broad signal; for ^{13}C{^{1}H} NMR spectra: s = quaternary carbon, d = CH carbon, t = CH_2 carbon and q = CH_3 carbon. ^{13}C NMR spectra are proton decoupled and interpreted with help of DEPT- and 2D spectra. All spectra were integrated and processed using Bruker TopSpin 4.1.1 software.

High-resolution mass spectra (HR-MS) were recorded at the chemistry department of Heidelberg University under the supervision of Dr. J. Gross on the following spectrometers: JEOL AccuTOF GCx (EI)**,** Bruker ApexQe hybrid 9.4 T FT-ICR (ESI, MALDI, DART), Finnigan LCQ (ESI), Bruker AutoFlex Speed (MALDI) and Bruker timsTOFfleX (ESI, MALDI).

Infrared spectra were recorded from a neat powder or oil on a FT-IR spectrometer (Bruker LUMOS) with a Germanium ATR-crystal. For the most significant bands the wave numbers are given.

UV-Vis spectra were recorded on a Jasco UV-VIS V-670. Fluorescence spectra were recorded on a Jasco FP6500. Quantum yields (QY) were recorded on a PTI QuantaMaster 40 with Ulbricht Sphere.

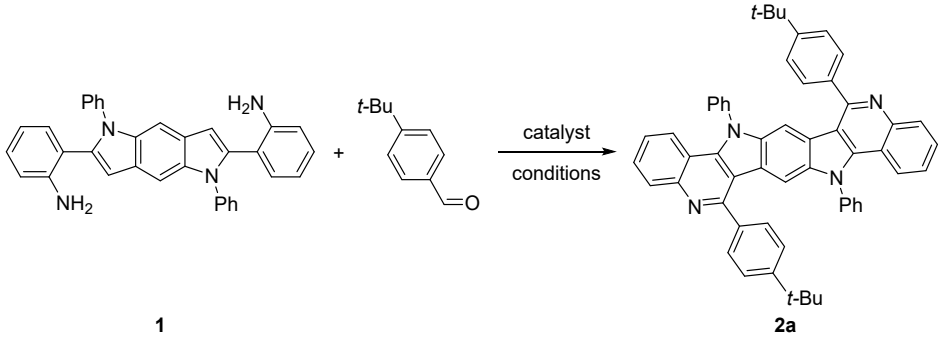
X-ray crystallography was carried out at the chemistry department of Heidelberg University under the supervision of Dr. F. Rominger on the following instruments: Bruker Smart APEX II Quazar (with Mo-microsource) and Stoe Stadivari (with Co-microsource and Pilatus detector). The structures were processed with Mercury 4.3.0.

For flash column chromatography silica gel (Sigma-Aldrich, pore size 60 Å, 70–230 mesh, 63–200 µm) or aluminum oxide (Honeywell, pore size 60 Å, activated, neutral) was used as stationary phase. As eluents different mixtures of petroleum ether (PE), ethyl acetate (EA), DCM or MeOH were used.

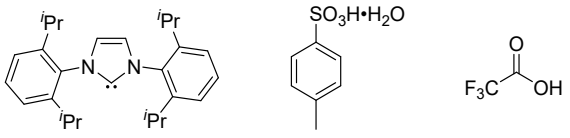
All reactions were performed under air, if not otherwise specified. For handling of air and moisture sensitive reagents, standard Schlenk techniques with flame-dried glassware under an argon or nitrogen atmosphere were used.

1.2 Catalyst Screening

Table S1. Optimization of the reaction conditions for the synthesis of **2a**.[a]



1 **2a**



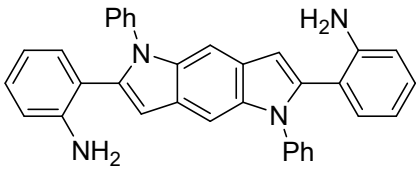
IPr PTSA•H_2O TFA

Entry	Catalyst	Solvent	Temperatur [°C]	Time	Yield[b] [%]
1	$IPrAuNTf_2$	MeCN	70	3 d	51
2	$IPrAuNTf_2$	DCE	80	2 d	65
3[c]	$IPrAuNTf_2$	DCE	80	3 d	-[c]
4	$Ph_3PAuNTf_2$	DCE	80	3 d	59
5	$AuCl_3$	DCE	80	3 d	42
	-	DCE	80	3 d	21
6	PTSA·H_2O	DCE	80	16 h	79
7	TFA	DCE	80	16 h	78

[a]The reactions were performed using **1** (15.0 mg, 30.6 µmol), 5eq. 4-(*tert*-butyl)benzaldehyde and 10 mol% catalyst in 2.0 mL of solvent. [b]Isolated yield. [c]Addition of molsieve; very low conversion after 3 d.

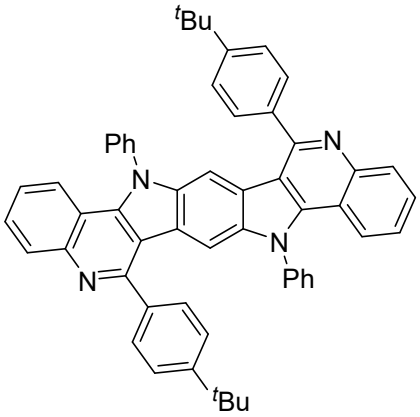
1.3 Synthesis of Compounds

2,2'-(1,5-Diphenyl-1,5-dihydropyrrolo[2,3-*f*]indole-2,6-diyl)dianiline (1)



1 was synthesized according to a literature procedure.[2]

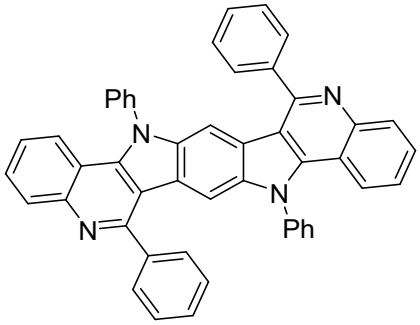
2a



1 (40.0 mg, 81.5 µmol), 4-*tert*-butylbenzaldehyde (39.7 mg, 245 µmol) and PTSA·H_2O (1.55 mg, 8.15 µmol) were dissolved in DCE (3 mL) and the mixture was stirred at 80 °C for 16 h. Pentane (3 mL) was added and the mixture was cooled to −20 °C for 1 h. The precipitate was filtered off and washed with MeOH and pentane. The product was obtained as a pale yellow solid (50.1 mg, 64.6 µmol, 79%).

Mp: >300 °C; **R_f**: 0.19 (silica gel, PE:EA = 5:1); **^{1}H NMR** (600 MHz, CD_2Cl_2, 32 °C): δ = 8.15 (d, *J* = 8.2 Hz, 2H), 7.81–7.79 (m, 4H), 7.72–7.69 (m, 6H), 7.62 (s, 2H), 7.61–7.58 (m, 2H), 7.56–7.54 (m, 4H), 7.47–7.45 (m, 4H), 7.29 (dd, *J* = 8.5 Hz, *J* = 0.9 Hz, 2H), 7.21–7.19 (m, 2H), 1.45 (s, 18H); **^{13}C{^{1}H} NMR** (151 MHz, CD_2Cl_2, 32 °C): δ = 156.3 (s, 2C), 152.4 (s, 2C), 147.3 (s, 2C), 142.9 (s, 2C), 139.6 (s, 2C), 139.4 (s, 2C), 138.4 (s, 2C), 130.9 (d, 4C), 130.6 (d, 2C), 130.2 (d, 2C), 129.6 (d, 4C), 129.1 (d, 4C), 128.4 (d, 2C), 125.5 (d, 4C), 125.1 (d, 2C), 122.5 (d, 2C), 121.8 (s, 2C), 116.9 (s, 2C), 113.5 (s, 2C), 102.9 (d 2C), 35.1 (s, 2C), 31.7 (q, 6C); **HR-MS** (MALDI+): *m/z* calculated for $[C_{56}H_{46}N_4]^+$, $[M]^+$: 774.3717, found: 774.3724; **IR** (ATR): ν [cm^{-1}] = 3064, 2964, 2902, 2866, 2196, 1599, 1561, 1499, 1433, 1362, 1340, 1268, 1220, 1196, 1105, 1072, 1027, 963, 927, 841, 761, 728, 701, 637, 609; **UV-Vis** (DCM): λ_{max} [nm] = 254, 327, 373, 388; **fluorescence** (DCM): λ_{ex} [nm] = 330, λ_{max} [nm] = 398, 420, 444, 472; **quantum yield** (DCM): Φ = 19%.

2b

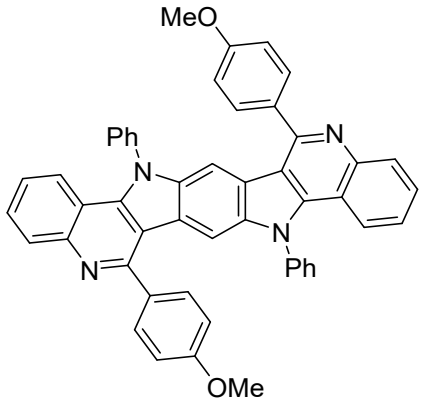


1 (40.0 mg, 81.5 µmol), benzaldehyde (26.0 mg, 245 µmol) and PTSA·H_2O (1.55 mg, 8.15 µmol) were dissolved in DCE (4 mL) and the mixture was stirred at 80 °C for 16 h. The solvent was removed under reduced pressure and the residue was recrystallized from hot EA and washed with MeOH and pentane. The product was obtained as a pale yellow solid (41.7 mg, 62.9 µmol, 77%).

Mp: >300 °C; **R_f**: 0.60 (silica gel, PE:EA = 1:1); **^{1}H NMR** (700 MHz, TCE-d_2, 100 °C): δ = 8.66 (br, 2H), 7.71–7.67 (m, 6H), 7.63–7.61 (m, 6H), 7.38–7.33 (m, 12H), 7.26 (t, *J* = 6.9 Hz, 2H), 6.97 (s, 2H); **^{13}C{^{1}H} NMR** (176 MHz, TCE-d_2, 100 °C): δ = 143.0 (s, 2C), 139.8 (s, 2C), 138.2 (s, 2C), 130.4 (d, 4C), 129.5 (d, 2C), 129.0 (d, 4C), 128.3 (d, 8C), 125.9 (s, 2C), 122.0 (d, 2C), 116.2 (s, 2C), 113.4 (s, 2C), 102.9 (d, 2C); **HR-MS** (MALDI+): *m/z* calculated for $[C_{48}H_{30}N_4]^+$, $[M]^+$: 662.2465, found: 662.2468; **IR** (ATR): ν [cm^{-1}] = 3054, 3031, 1909, 1626, 1595, 1556, 1491, 1431, 1341, 1327, 1294, 1265, 1218, 1199, 1161, 1109, 1073, 1025, 985, 959, 936, 921, 902, 869, 845, 835, 796, 761, 732, 725, 705, 695, 664, 631, 624, 612; **UV-Vis** (DCM): λ_{max} [nm] = 257, 327, 370, 387; **fluorescence** (DCM): λ_{ex} [nm] = 325, λ_{max} [nm] = 397, 419, 443, 471, 511; **quantum yield** (DCM): Φ = 15%.

Not all carbon peaks could be determined in ^{13}C{^{1}H} NMR due to low solubility.

2c



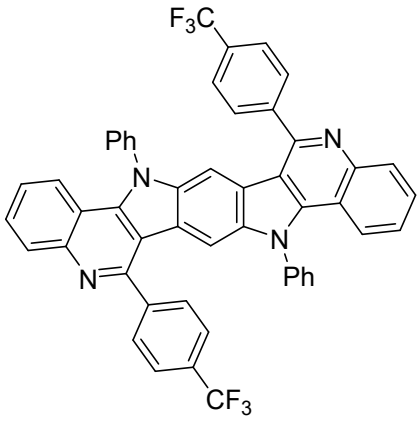
1 (50.0 mg, 102 µmol), 4-methoxybenzaldehyde (41.6 mg, 306 µmol) and PTSA·H_2O (1.94 mg, 10.2 µmol) were dissolved in DCE (3 mL) and the mixture was stirred at 80 °C for 16 h. Pentane (3 mL) was added and the mixture was cooled to −20 °C for 1 h. The precipitate was filtered off and

washed with MeOH, EA and pentane. The product was obtained as a pale yellow solid (57.5 mg, 79.6 mmol, 78%).

Mp: >300 °C; **R_f**: 0.21 (silica gel, PE:EA = 1:1); **^{1}H NMR** (301 MHz, TCE-d_2): δ = 8.25 (d, *J* = 8.3 Hz, 2H), 7.72–7.63 (m, 12H), 7.51–7.44 (m, 6H), 7.29 (t, *J* = 7.7 Hz, 2H), 7.16 (s, 2H), 6.93 (d, *J* = 8.5 Hz, 4H), 3.96 (s, 6H); **^{13}C{^{1}H} NMR** (176 MHz, TCE-d_2, 140 °C): δ = 130.9 (d, 4C), 130.4 (d, 4C), 129.9 (d, 2C), 128.2 (d, 4C), 126.2 (d, 2C), 123.7 (d, 2C), 121.9 (d, 2C), 120.2 (d, 2C), 114.3 (d, 4C), 103.3 (d, 2C), 55.4 (q, 2C); **HR-MS** (DART+): *m/z* calculated for $[C_{50}H_{35}N_4O_2]^+$, $[M+H]^+$: 723.2755, found: 723.2748; **IR** (ATR): ν [cm^{-1}] = 3072, 2932, 2837, 1634, 1607, 1586, 1556, 1502, 1433, 1355, 1339, 1300, 1247, 1198, 1167, 1118, 1074, 1030, 1009, 932, 904, 842, 816, 793, 764, 736, 710, 696, 680, 638, 616; **UV-Vis** (DCM): λ_{max} [nm] = 263, 327, 371, 386; **fluorescence** (DCM): λ_{ex} [nm] = 330, λ_{max} [nm] = 396, 419, 442; **quantum yield** (DCM): Φ = 22%.

Quaternary carbons could be not determined in ^{13}C{^{1}H} NMR due to low solubility.

2d

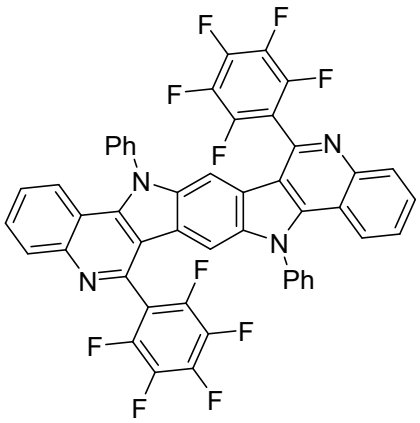


1 (30.0 mg, 61.2 µmol), 4-(trifluoromethyl)benzaldehyde (31.9 mg, 183 µmol) and PTSA·H_2O (1.16 mg, 6.11 µmol) were dissolved in DCE (2 mL) and the mixture was stirred at 80 °C for 16 h. Pentane (2 mL) was added and the mixture was cooled to −20 °C for 1 h. The precipitate was filtered off and washed with MeOH, EA and pentane. The product was obtained as a pale yellow solid (36.1 mg, 45.3 µmol, 74%).

Mp: >300 °C; **R_f**: 0.27 (silica gel, PE:EA = 5:1); **^{1}H NMR** (700 MHz, TCE-d_2): δ = 8.26 (d, *J* = 8.0 Hz, 2H), 7.94 (d, *J* = 7.6 Hz, 4H), 7.73 (t, *J* = 7.5 Hz, 2H), 7.70–7.68 (m, 10H), 7.48–7.47 (m, 6H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.13 (s, 2H); **^{13}C{^{1}H} NMR** (176 MHz, TCE-d_2): δ = 154.2 (s, 2C), 146.4 (s, 2C), 143.9 (s, 2C), 142.1 (s, 2C), 139.1 (s, 2C), 138.0 (s, 2C), 130.3 (d, 4C), 130.2 (d, 2C), 129.8 (d, 2C), 129.5 (d, 4C), 128.5 (d, 2C), 128.4 (d, 4C), 125.5 (d, 2C), 125.2 (d, 4C), 124.0 (s, *J* = 272 Hz, $2CF_3$), 122.1 (d, 2C), 120.7 (s, 2C), 120.2 (s, 2C), 116.6 (s, 2C), 112.8 (s, 2C), 102.0 (d, 2C); **^{19}F{^{1}H} NMR** (283 MHz; TCE-d_2): δ = −61.6 (6F); **HR-MS** (DART+): *m/z* calculated for $[C_{50}H_{29}F_6N_4]^+$, $[M+H]^+$: 799.2291, found: 799.2279; **IR** (ATR): ν [cm^{-1}] = 3028, 1600, 1564, 1501, 1459, 1439, 1408, 1323, 1225, 1164, 1122, 1106, 1065, 1020, 965, 925, 853, 780, 759, 735, 726, 699, 680, 640, 608; **UV-Vis**

(DCM): λ_{max} [nm] = 264, 327, 373, 389; **fluorescence** (DCM): λ_{ex} [nm] = 370, λ_{max} [nm] = 416; **quantum yield** (DCM): Φ = 17%.

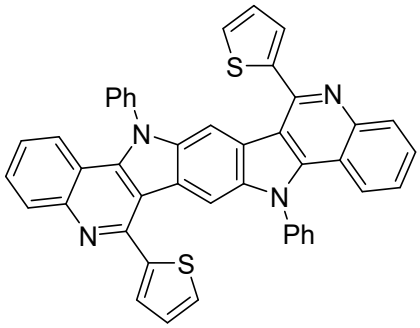
2e



1 (25.0 mg, 51.0 µmol), pentafluorobenzaldehyde (30.0 mg, 153 µmol) and PTSA·H_2O (969 µg, 5.10 µmol) were dissolved in DCE (2 mL) and the mixture was stirred at 80 °C for 16 h. Pentane (2 mL) was added and the mixture was cooled to −20 °C for 1 h. The precipitate was filtered off and washed with MeOH and pentane. The product was obtained as a pale yellow solid (31.2 mg, 37.0 µmol, 73%).

Mp: >300 °C; **R_f**: 0.87 (silica gel, PE:EA = 1:1); **^{1}H NMR** (301 MHz, $CDCl_3$): δ = 8.25 (dd, *J* = 8.5 Hz, *J* = 0.6 Hz, 2H), 7.81–7.73 (m, 6H), 7.72–7.66 (m, 2H), 7.61–7.58 (m, 2H), 7.54–7.51 (m, 4H), 7.38–7.33 (m, 2H), 6.61 (s, 2H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$): δ = 146.9 (s, 2C), 144.9 (s, *J* = 251 Hz, 4CF), 142.1 (s, 2C), 141.7 (s, *J* = 266 Hz, 2CF), 141.6 (s, 2C), 139.8 (s, 2C), 138.4 (s, 2C), 138.2 (s, 2C), 138.0 (s, *J* = 246 Hz, 4CF), 130.8 (d, 2C), 130.6 (d, 4C), 130.1 (d, 2C), 129.0 (d, 2C), 128.9 (d, 4C), 126.5 (d, 2C), 122.3 (d, 2C), 120.5 (s, 2C), 117.2 (s, 2C), 114.4 (s, 2C), 100.5 (d, 2C); **^{19}F{^{1}H} NMR** (471 MHz; $CDCl_3$): δ = −140.3 (dd, *J* = 22.9 Hz, *J* = 8.2 Hz, 4F), −152.8 (t, *J* = 20.9 Hz, 2F), −161.0 (td, *J* = 21.8 Hz, *J* = 8.4 Hz, 4F); **HR-MS** (ESI+): *m/z* calculated for $[C_{48}H_{21}F_{10}N_4]^+$, $[M+H]^+$: 843.1601, found: 843.1617; **IR** (ATR): ν [cm^{-1}] = 2921, 1737, 1562, 1495, 1434, 1341, 1304, 1269, 1192, 1153, 1104, 1079, 1027, 986, 905, 878, 848, 756, 701, 622; **UV-Vis** (DCM): λ_{max} [nm] = 254, 319, 330, 372, 385; **fluorescence** (DCM): λ_{ex} [nm] = 370, λ_{max} [nm] = 396, 418, 440; **quantum yield** (DCM): Φ = 30%.

2f

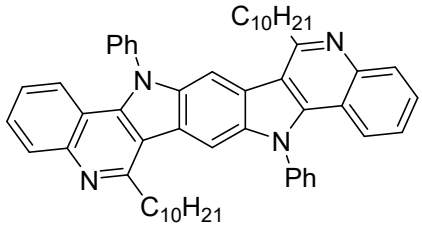


1 (25.0 mg, 51.0 µmol), thiophene-2-carboxaldehyde (17.1 mg, 153 µmol) and PTSA·H_2O (969 µg, 5.10 µmol) were dissolved in DCE (2 mL) and the mixture was stirred at 80 °C for 16 h. Pentane (2 mL) was added and the mixture was cooled to −20 °C for 1 h. The precipitate was filtered off and washed with MeOH and pentane. The product was obtained as a pale yellow solid (18.6 mg, 27.6 µmol, 54%).

Mp: >300 °C; $\mathbf{R_f}$: 0.71 (silica gel, PE:EA = 1:1); **^{1}H NMR** (500 MHz, TCE-d_2, 80 °C): δ = 8.46 (br, 2H), 7.79–7.78 (m, 6H), 7.73–7.70 (m, 2H), 7.63–7.50 (m, 12H), 7.36–7.33 (m, 2H), 7.08 (br, 2H); **^{13}C{^{1}H} NMR** (176 MHz, TCE-d_2, 140 °C): δ = 130.3 (d, 4C), 129.7 (d, 2C), 129.4 (d, 2C), 129.2 (d, 2C), 128.5 (d, 4C), 128.2 (d, 2C), 128.1 (d, 2C), 126.8 (d, 2C), 126.0 (d, 2C), 121.9 (d, 2C), 103.0 (d, 2C); **HR-MS** (ESI+): *m/z* calculated for $[C_{44}H_{27}N_4S_2]^+$, $[M+H]^+$: 675.1672, found: 675.1683; **IR** (ATR): ν [cm^{-1}] = 3066, 2927, 2854, 1738, 1673, 1557, 1498, 1434, 1341, 1313, 1267, 1218, 1198, 1108, 1074, 928, 902, 855, 839, 761, 736, 707, 628; **UV-Vis** (DCM): λ_{max} [nm] = 253, 328, 374, 391; **fluorescence** (DCM): λ_{ex} [nm] = 330, λ_{max} [nm] = 418, 433, 506; **quantum yield** (DCM): Φ = 5%.

Quaternary carbons could be not determined in ^{13}C{^{1}H} NMR due to low solubility.

2g

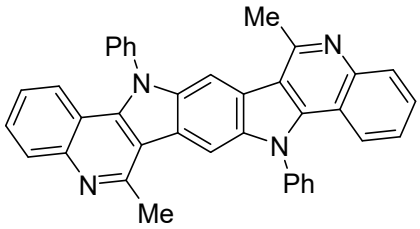


1 (30.0 mg, 61.2 µmol), undecanal (31.2 mg, 183 µmol) and PTSA·H_2O (1.16 mg, 6.11 µmol) were dissolved in DCE (2 mL) and the mixture was stirred at 80 °C for 16 h. The solvent was removed under reduced pressure and the residue was filtered through a plug of aluminum oxide (eluted with PE:EA = 2:1, 5 mL). Pentane (2 mL) was added and the mixture was cooled to −20 °C for 1 h. The precipitate was filtered off and washed with MeOH and pentane. The product was obtained as a pale yellow solid (32.0 mg, 40.5 µmol, 66%).

Mp: 204–206 °C; $\mathbf{R_f}$: 0.81 (silica gel, PE:EA = 1:1); **^{1}H NMR** (700 MHz, CD_2Cl_2): δ = 8.10 (d, *J* = 8.1 Hz, 2H), 7.86 (s, 2H), 7.80–7.78 (m, 6H), 7.68–7.67 (m, 4H), 7.60–7.58 (m, 2H), 7.40 (d, *J* = 8.3

Hz, 2H), 7.21 (t, *J* = 7.5 Hz, 2H), 3.35 (t, *J* = 8.4 Hz, 4H), 1.88–1.83 (m, 4H), 1.38–1.27 (m, 28H), 0.90 (t, *J* = 6.8 Hz, 6H); **$^{13}C\{^{1}H\}$ NMR** (176 MHz, CD_2Cl_2): δ = 159.2 (s, 2C), 147.1 (s, 2C), 142.2 (s, 2C), 139.9 (s, 2C), 139.5 (s, 2C), 131.0 (d, 4C), 130.1 (d, 2C), 129.9 (d, 2C), 129.6 (d, 4C), 128.2 (d, 2C), 124.7 (d, 2C), 122.5 (d, 2C), 121.3 (s, 2C), 117.0 (s, 2C), 113.9 (s, 2C), 102.6 (d, 2C), 39.1 (t, 2C), 32.4 (t, 2C), 30.7 (t, 2C), 30.1 (t, 4C), 30.1 (t, 2C), 29.9 (t, 2C), 28.9 (t, 2C), 23.1 (t, 2C), 14.3 (q, 2C); **HR-MS** (DART+): *m/z* calculated for $[C_{56}H_{63}N_4]^+$, $[M+H]^+$: 791.5047, found: 791.5030; **IR** (ATR): ν [cm^{-1}] = 3063, 2952, 2921, 2849, 1597, 1560, 1500, 1433, 1339, 1269, 1232, 1193, 1102, 1030, 1004, 929, 901, 859, 840, 786, 756, 727, 699, 622; **UV-Vis** (DCM): λ_{max} [nm] = 257, 310, 319, 347, 367, 383; **fluorescence** (DCM): λ_{ex} [nm] = 320, λ_{max} [nm] = 388, 410, 434, 464; **quantum yield** (DCM): Φ = 46%.

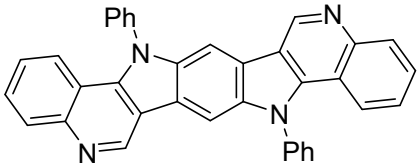
2h



1 (20.0 mg, 40.8 µmol), acetaldehyde (44.9 mg, 1.02 mmol) and PTSA·H_2O (775 µg, 4.08 µmol) were dissolved in DCE (2 mL) and the mixture was stirred at 80 °C for 16 h. Pentane (2 mL) was added and the mixture was cooled to −20 °C for 1 h. The precipitate was filtered off and washed with MeOH, EA and pentane. The product was obtained as a pale yellow solid (18.2 mg, 33.8 µmol, 83%).

Mp: >300 °C; **R_f**: 0.15 (silica gel, PE:EA = 1:1); **^{1}H NMR** (700 MHz, TCE-d_2): δ = 8.22 (br, 2H), 7.97 (s, 2H), 7.84–7.81 (m, 6H), 7.69 (d, *J* = 6.5 Hz, 4H), 7.65 (t, *J* = 7.2 Hz, 2H), 7.34 (d, *J* = 8.3 Hz, 2H), 7.28 (t, *J* = 7.4 Hz, 2H), 3.16 (s, 6H); **$^{13}C\{^{1}H\}$ NMR** (176 MHz, TCE-d_2): δ = 154.5 (s, 2C), 146.0 (s, 2C), 141.5 (s, 2C), 139.1 (s, 2C), 138.3 (s, 2C), 130.7 (d, 4C), 130.0 (d, 2C), 129.0 (d, 2C), 128.9 (d, 4C), 128.2 (d, 2C), 124.8 (d, 2C), 122.0 (d, 2C), 120.2 (s, 2C), 116.3 (s, 2C), 113.9 (s, 2C), 102.3 (d, 2C), 24.8 (q, 2C); **HR-MS** (DART+): *m/z* calculated for $[C_{38}H_{27}N_4]^+$, $[M+H]^+$: 539.2230, found: 539.2225; **IR** (ATR): ν [cm^{-1}] 3058, 2991, 2928, 1954, 1597, 1562, 1500, 1455, 1437, 1425, 1362, 1341, 1278, 1232, 1207, 1189, 1158, 1104, 1073, 1034, 999, 928, 904, 870, 835, 758, 728, 699, 679, 655, 622, 607; **UV-Vis** (DCM): λ_{max} [nm] = 256, 309, 317, 346, 365, 381; **fluorescence** (DCM): λ_{ex} [nm] = 345, λ_{max} [nm] = 389, 409, 432, 461; **quantum yield** (DCM): Φ = 37%.

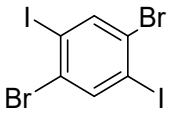
2i



1 (30.0 mg, 61.2 µmol), formaldehyde (5.51 mg, 183 µmol) and PTSA·H_2O (1.16 mg, 6.11 µmol) were dissolved in DCE (2 mL) and the mixture was stirred at 80 °C for 16 h. Pentane (2 mL) was added and the mixture was cooled to −20 °C for 1 h. The precipitate was filtered off and washed with MeOH and pentane. The product was obtained as a pale yellow solid (19.5 mg, 38.2 µmol, 62%).

Mp: >300 °C; **R_f**: 0.15 (silica gel, PE:EA = 1:1); **^{1}H NMR** (301 MHz, CD_2Cl_2): δ = 9.57 (s, 2H), 8.21 (d, *J* = 8.9 Hz, 2H), 8.02 (s, 2H), 7.83–7.82 (m, 6H), 7.72–7.61 (m, 6H), 7.43 (d, *J* = 8.2 Hz, 2H), 7.29 (t, *J* = 7.8 Hz, 2H) **^{13}C{^{1}H} NMR** (151 MHz, CD_2Cl_2, 32 °C): δ = 147.4 (s, 2C), 144.6 (d, 2C), 141.9 (s, 2C), 139.9 (s, 2C), 139.3 (s, 2C), 131.1 (d, 4C), 130.5 (d, 2C), 130.3 (d, 2C), 129.6 (d, 4C), 128.4 (d, 2C), 125.7 (d, 2C), 122.6 (d, 2C), 122.3 (s, 2C), 117.9 (s, 2C), 115.8 (s, 2C), 100.8 (d, 2C); **HR-MS** (DART+): *m/z* calculated for $[C_{36}H_{23}N_4]^+$, $[M+H]^+$: 511.1917, found: 511.1913; **IR** (ATR): ν [cm^{-1}] = 3049, 1586, 1563, 1501, 1435, 1384, 1358, 1315, 1264, 1190, 1152, 1108, 1074, 1062, 1029, 930, 898, 844, 794, 753, 718, 699, 677, 621; **UV-Vis** (DCM): λ_{max} [nm] = 256, 313, 323, 345, 367, 380; **fluorescence** (DCM): λ_{ex} [nm] = 370, λ_{max} [nm] = 387, 410, 432, 462; **quantum yield** (DCM): Φ = 39%.

1,4-Dibromo-2,5-diiodobenzene (S1)

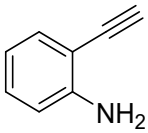


1,4-Dibromobenzene (19.9 g, 84.3 mmol) was dissolved in 200 mL concentrated sulfuric acid, then, iodine (86.2 g, 340 mmol) was added in portions. The mixture was stirred at 115 °C for 1 d, cooled, poured on ice and extracted with DCM. The combined organic layers were washed with aqueous NaOH and the solvent was removed under reduced pressure. The residue was dissolved in refluxing chloroform (150 mL), then, methanol (100 mL) was added and the mixture was cooled to −20 °C for 1 h. The precipitate was filtered off and washed with methanol. The product was obtained as a colorless solid (24.2 g, 49.6 mmol, 59%).

R_f: 0.79 (silica gel, PE:EA = 20:1); **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 8.05 (s, 2H).

The spectroscopic data correspond to those previously reported in the literature.[3]

2-Ethynylaniline (S2)

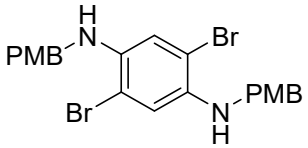


A Schlenk flask containing 2-iodoaniline (8.00 g, 35.5 mmol) and $Pd(PPh_3)_2Cl_2$ (256 mg, 365 µmol) was evacuated and refilled with nitrogen three times. Degassed Et_3N (150 mL) and ethynyltrimethylsilane (4.48 g, 45.7 mmol) were added and the mixture was stirred at rt for 5 min. CuI (139 mg, 731 µmol) was added and the mixture was stirred at rt for 2 h. The mixture was filtered through a plug of Celite® (eluted with EA), the solvents were removed under reduced pressure and the residue was dissolved in methanol (150 mL). K_2CO_3 (10.1 g, 73.1 mmol) was added and the resulting mixture was stirred at rt for 30 min. The solvent was removed under reduced pressure and the residue was purified by flash column chromatography (silica gel, PE:EA = 20:1 to 5:1). The product was obtained as a pale yellow oil (3.06 g, 26.1 mmol, 74%).

R_f: 0.24 (silica gel, PE:EA = 10:1); **^{1}H NMR** (301 MHz, $CDCl_3$): δ = 7.32 (dd, *J* = 7.7 Hz, *J* = 1.2 Hz, 1H), 7.17–7.12 (m, 1H), 6.71–6.65 (m, 2H), 4.24 (br, 2H), 3.38 (s, 1H).

The spectroscopic data correspond to those previously reported in the literature.[4]

2,5-Dibromo-*N*^{1},*N*^{4}-bis(4-methoxybenzyl)benzene-1,4-diamine (3)

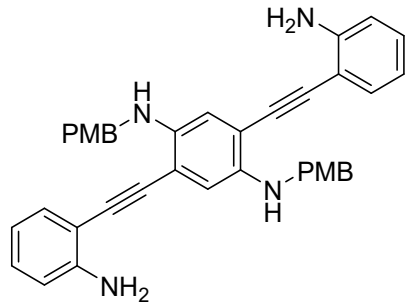


A Schlenk flask containing **S1** (2.00 g, 4.10 mmol), NaO^{t}Bu (1.18 g, 12.3 mmol), $Pd_2(dba)_3$ (93.9 mg, 103 µmol) and *rac*-BINAP (128 mg, 205 µmol) was evacuated and refilled with argon three times. Then, degassed toluene (50 mL) and 4-methoxybenzylamine (1.69 g, 12.3 mmol) were added and the resulting mixture was stirred at 115 °C for 3 d. The mixture was filtered through a plug of Celite® (eluted with EA) and the solvents were removed under reduced pressure. The residue was purified by flash column chromatography (silica gel, PE:EA = 40:1 to PE:DCM = 5:1 to DCM). The product was obtained as an off-white solid (1.79 g, 3.54 mmol, 86%).

R_f: 0.40 (silica gel, PE:EA = 5:1); **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 7.29–7.26 (m, 4H), 6.90–6.87 (m, 4H), 6.83 (s, 2H), 4.22 (s, 4H), 4.11 (br, 2H), 3.81 (s, 6H).

The spectroscopic data correspond to those previously reported in the literature.[5]

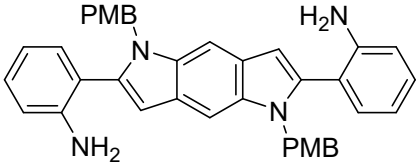
2,5-Bis((2-aminophenyl)ethynyl)-*N*^{1},*N*^{4}-bis(4-methoxybenzyl)benzene-1,4-diamine (4)



A Schlenk flask containing **3** (500 mg, 988 µmol) and $Pd(PPh_3)_2Cl_2$ (34.7 mg, 49.4 µmol) was evacuated and refilled with argon three times. Degassed Et_3N (15 mL) and **S2** (347 mg, 2.96 mmol) were added and the mixture was stirred at rt for 5 min. CuI (18.8 mg, 98.8 µmol) was added and the mixture was stirred at 90 °C for 16 h. The solvent was removed under reduced pressure, then, water was added and the mixture was extracted with EA. The combined organic layers were washed with water and brine, dried over Na_2SO_4 and the solvent was removed under reduced pressure. The product partly cyclized during the reaction and was therefore used without further purification in the next step.

R_f: 0.76 (silica gel, PE:EA = 1:1).

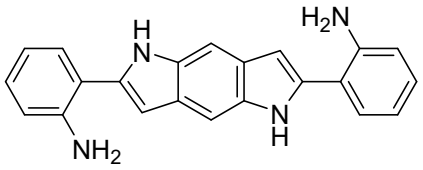
2,2'-(1,5-Bis(4-methoxybenzyl)-1,5-dihydropyrrolo[2,3-*f*]indole-2,6-diyl)dianiline (5)



The crude product **4** (theoretical yield: 988 µmol) and IPrAuNTf$_2$ (43.2 mg, 49.9 µmol) were dissolved in DCM (20 mL) and the mixture was stirred at rt for 6 h. MeOH (40 mL) was added, the resulting precipitate was filtered off, washed with MeOH and recrystallized from DCM/pentane. The product was obtained as a pale yellow solid (441 mg, 762 µmol, 77% over two steps).

Mp: 259–263 °C; **R_f**: 0.68 (silica gel, PE:EA = 1:1); **^{1}H NMR** (600 MHz, DMSO-d_6): δ = 7.38 (s, 2H), 7.12–7.08 (m, 4H), 6.86 (d, *J* = 8.2 Hz, 4H), 6.80 (d, *J* = 7.9 Hz, 2H), 6.73 (d, *J* = 8.3 Hz, 4H), 6.61 (t, *J* = 7.2 Hz, 2H), 6.44 (s, 2H), 5.17 (s, 4H), 4.95 (s, 4H), 3.64 (s, 6H); **^{13}C{^{1}H} NMR** (151 MHz, DMSO-d_6): δ = 158.1 (s, 2C), 146.8 (s, 2C), 138.9 (s, 2C), 133.9 (s, 2C), 131.1 (d, 2C), 130.5 (s, 2C), 129.3 (d, 2C), 127.5 (d, 4C), 125.7 (s, 2C), 116.5 (s, 2C), 116.0 (d, 2C), 114.9 (d, 2C), 113.7 (d, 4C), 100.9 (d, 2C), 99.7 (d, 2C), 54.9 (q, 2C), 46.2 (t, 2C); **HR-MS** (DART+): *m/z* calculated for $[C_{38}H_{35}N_4O_2]^+$, $[M+H]^+$: 579.2755, found: 579.2778; **IR** (ATR): ν [cm^{-1}] = 3444, 3359, 3010, 2968, 2935, 2907, 2835, 1875, 1614, 1574, 1510, 1479, 1454, 1406, 1369, 1344, 1299, 1246, 1225, 1176, 1104, 1026, 876, 826, 813, 757, 747, 710, 670.

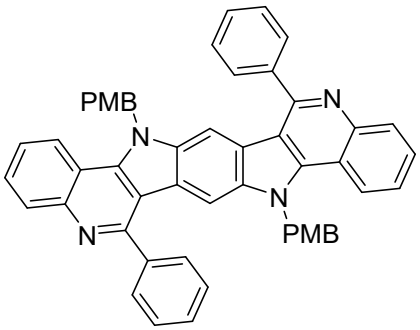
2,2'-(1,5-Dihydropyrrolo[2,3-*f*]indole-2,6-diyl)dianiline (6)



5 (390 mg, 674 µmol) and $AlCl_3$ (899 mg, 6.74 mmol) were added to a flame-dried Schlenk flask containing anhydrous toluene (10 mL) under an atmosphere of nitrogen and the mixture was stirred at 80 °C for 16 h. A saturated aqueous solution of $NaHCO_3$ was added and the mixture was extracted with EA. The combined organic layers were washed with water and brine, dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was filtered through a plug of aluminum oxide, eluted with EA and THF and the solvents were removed under reduced pressure. 209 mg of a crude product containing unknown impurities was obtained, which seemed to be not fully stable and therefore a complete characterization was not possible.

R_f: 0.75 (silica gel, PE:EA = 1:1); **^{1}H NMR** (301 MHz, DMSO-d_6): δ = 10.70 (s, 2H), 7.44 (s, 2H), 7.42–7.39 (m, 2H), 7.07–7.02 (m, 2H), 6.87 (s, 2H), 6.84–6.81 (m, 2H), 6.71–6.67 (m, 2H), 5.20 (br, 4H); **HR-MS** (EI+): *m/z* calculated for $[C_{22}H_{18}N_4]^+$, $[M]^+$: 338.15260, found: 338.15346.

7a

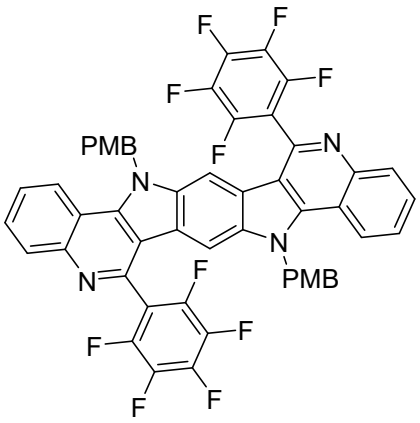


5 (40.0 mg, 69.1 µmol), benzaldehyde (22.0 mg, 207 µmol) and PTSA·H_2O (1.31 mg, 6.91 µmol) were dissolved in DCE (3 mL) and the mixture was stirred at 80 °C for 16 h. A saturated aqueous solution of $NaHCO_3$ was added and the mixture was extracted with DCM. The combined organic layers were washed with water and brine, dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was washed with MeOH and recrystallized from DCM/pentane. The product was obtained as a pale yellow solid (38.6 mg, 51.4 µmol, 74%).

Mp: decomposition >280 °C; **R_f**: 0.43 (silica gel, PE:EA = 1:1); **^{1}H NMR** (600 MHz, $CDCl_3$): δ = 8.35–8.32 (m, 4H), 7.76 (d, *J* = 7.3 Hz, 4H), 7.70 (t, *J* = 7.5 Hz, 2H), 7.55 (t, *J* = 7.5 Hz, 2H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.46–7.43 (m, 4H), 7.37 (s, 2H), 7.09 (d, *J* = 8.7 Hz, 4H), 6.88 (d, *J* = 8.6 Hz, 4H), 5.77 (br, 4H), 3.81 (s, 6H); **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ = 159.3 (s, 2C), 156.3 (s, 2C), 146.9 (s, 2C), 142.2 (s, 2C), 141.0 (s, 2C), 137.5 (s, 2C), 130.9 (d, 2C), 129.0 (d, 4C), 128.9 (d, 2C), 128.8 (d, 4C), 128.4 (d, 2C), 128.2 (s, 2C), 127.6 (d, 4C), 125.7 (d, 2C), 121.9 (d, 2C), 121.6 (s, 2C), 116.9 (s, 2C), 114.5 (d, 4C), 113.4 (s, 2C), 101.8 (d, 2C), 55.5 (q, 2C), 49.5 (t, 2C); **HR-MS** (ESI+): *m/z* calculated for

$[C_{52}H_{39}N_4O_2]^+$, $[M+H]^+$: 751.3068, found: 751.3073; **IR** (ATR): ν [cm^{-1}] = 3365, 3064, 2954, 2932, 2833, 1613, 1586, 1557, 1512, 1493, 1440, 1342, 1302, 1269, 1249, 1216, 1174, 1152, 1126, 1072, 1024, 948, 889, 833, 813, 796, 754, 733, 702, 673, 638, 628; **UV-Vis** (DCM): λ_{max} [nm] 264, 329, 374, 389; **fluorescence** (DCM): λ_{ex} [nm] = 390, λ_{max} [nm] = 401, 424, 447; **quantum yield** (DCM): Φ = 15%.

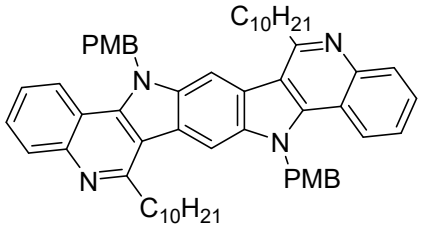
7b



5 (20.0 mg, 34.6 µmol), pentafluorobenzaldehyde (20.3 mg, 104 µmol) and PTSA·H_2O (657 µg, 3.46 µmol) were dissolved in DCE (2 mL) and the mixture was stirred at 80 °C for 16 h. A saturated aqueous solution of $NaHCO_3$ was added and the mixture was extracted with DCM. The combined organic layers were washed with water and brine, dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was washed with MeOH and recrystallized from DCM/pentane. The product was obtained as a pale yellow solid (22.8 mg, 24.5 µmol, 71%).

Mp: >300 °C; $\mathbf{R_f}$: 0.10 (silica gel, PE:EA = 1:1); **^{1}H NMR** (600 MHz, $CDCl_3$, 50 °C): δ = 8.38–8.37 (m, 4H), 7.79 (t, *J* = 7.5 Hz, 2H), 7.62 (t, *J* = 7.6 Hz, 2H), 7.17–7.15 (m, 6H), 6.96 (d, *J* = 8.7 Hz, 4H), 5.90 (s, 4H), 3.85 (s, 6H); **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$, 50 °C): δ = 168.8 (s, 2C), 160.0 (s, 2C), 147.0 (s, 2H), 145.4 (s, 2C), 145.0 (s, *J* = 251 Hz, 4CF), 143.1 (s, 2C), 142.1 (s, *J* = 252 Hz, 2CF), 141.2 (s, 2C), 138.5 (s, 2C), 138.2 (s, *J* = 251 Hz, 4CF), 131.2 (d, 2C), 129.1 (d, 2C), 127.2 (d, 2C), 126.9 (d, 4C), 122.0 (d, 2C), 121.3 (s, 2C), 117.3 (s, 2C), 115.2 (d, 4C), 114.6 (s, 2C), 100.6 (d, 2C), 55.5 (q, 2C), 50.5 (t, 2C); **^{19}F{^{1}H} NMR** (283 MHz; $CDCl_3$): δ = −140.2 (dd, *J* = 23.2 Hz, *J* = 8.5 Hz, 4F), −152.7 (t, *J* = 21.4 Hz, 2F), −160.6–(−160.8) (m, 4F); **HR-MS** (DART+): *m/z* calculated for $[C_{52}H_{29}F_{10}N_4O_2]^+$, $[M+H]^+$: 931.2125, found: 931.2140; **IR** (ATR): ν [cm^{-1}] = 2944, 2842, 1656, 1614, 1567, 1515, 1496, 1446, 1341, 1306, 1286, 1254, 1177, 1148, 1126, 1080, 1031, 984, 895, 878, 833, 820, 807, 754, 684; **UV-Vis** (DCM): λ_{max} [nm] = 262, 322, 330, 375, 389; **fluorescence** (DCM): λ_{ex} [nm] = 375, λ_{max} [nm] = 399, 421, 443; **quantum yield** (DCM): Φ = 24%.

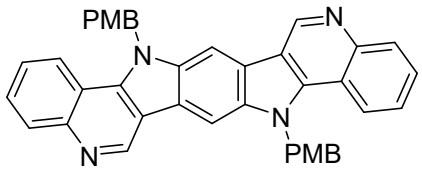
7c



5 (40.0 mg, 69.1 µmol), undecanal (35.3 mg, 207 µmol) and PTSA·H_2O (1.31 mg, 6.91 µmol) were dissolved in DCE (2 mL) and the mixture was stirred at 80 °C for 16 h. A saturated aqueous solution of $NaHCO_3$ was added and the mixture was extracted with DCM. The combined organic layers were washed with water and brine, dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was washed with MeOH and recrystallized from DCM/pentane. The product was obtained as a pale yellow solid (44.1 mg, 50.2 µmol, 73%).

Mp: decomposition >270 °C; $\mathbf{R_f}$: 0.41 (silica gel, PE:EA = 1:1); **^{1}H NMR** (301 MHz, CD_2Cl_2): δ = 8.32 (d, *J* = 8.5 Hz, 2H), 8.24 (s, 2H), 8.16 (d, *J* = 8.4 Hz, 2H), 7.66 (t, *J* = 7.3 Hz, 2H), 7.44 (d, *J* = 7.1 Hz, 2H), 7.25 (d, *J* = 8.2 Hz, 4H), 6.88 (d, *J* = 8.5 Hz, 4H), 6.12 (s, 4H), 3.75 (s, 6H), 3.50 (t, *J* = 7.9 Hz, 4H), 1.94 (quint, *J* = 7.7 Hz, 4H), 1.58–1.50 (m, 4H), 1.27 (br, 24H), 0.89 (t, *J* = 6.9 Hz, 6H); **^{13}C{^{1}H} NMR** (151 MHz, CD_2Cl_2): δ = 159.7 (s, 2C), 159.0 (s, 2C), 147.1 (s, 2C), 142.1 (s, 2C), 138.3 (s, 2C), 130.2 (d, 2C), 128.8 (s, 2C), 128.2 (d, 2C), 127.5 (d, 4C), 125.1 (d, 2C), 122.3 (d, 2C), 121.5 (s, 2C), 117.0 (s, 2C), 114.9 (d, 4C), 113.7 (s, 2C), 101.9 (d, 2C), 55.6 (q, 2C), 49.8 (t, 2C), 38.9 (t, 2C), 32.4 (t, 2C), 30.7 (t, 2C), 30.1 (t, 2C), 30.1 (t, 2C), 30.1 (t, 2C), 29.8 (t, 2C), 28.8 (t, 2C), 23.1 (t, 2C), 14.3 (q, 2C); **HR-MS** (ESI+): *m/z* calculated for $[C_{60}H_{71}N_4O_2]^+$, $[M+H]^+$: 879.5572, found: 879.5587; **IR** (ATR): ν [cm^{-1}] = 2921, 2851, 1615, 1561, 1513, 1467, 1442, 1342, 1294, 1247, 1175, 1146, 1108, 1034, 977, 889, 830, 753, 722, 670, 615; **UV-Vis** (DCM): λ_{max} [nm] = 263, 310, 319, 350, 371, 387; **fluorescence** (DCM): λ_{ex} [nm] = 350, λ_{max} [nm] = 392, 416, 440, 468; **quantum yield** (DCM): Φ = 43%.

7d

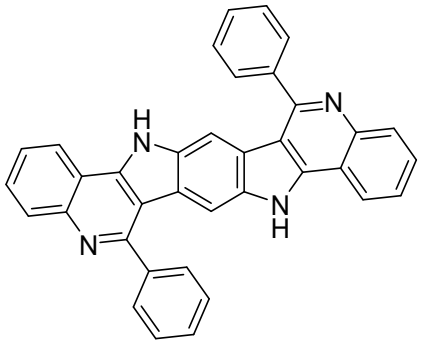


5 (40.0 mg, 69.1 µmol), *N*,*N*-dimethylformamide dimethyl acetal (24.7 mg, 207 µmol) and PTSA·H_2O (1.31 mg, 6.91 µmol) were dissolved in DCE (5 mL) and the mixture was stirred at 80 °C for 16 h. A saturated aqueous solution of $NaHCO_3$ was added and the mixture was extracted with DCM. The combined organic layers were washed with water and brine, dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was washed with MeOH and recrystallized from DCM/pentane. The product was obtained as a pale yellow solid (15.8 mg, 26.4 µmol, 38%).

Mp: decomposition >250 °C; **R_f**: 0.30 (silica gel, EA); **^{1}H NMR** (700 MHz, $CDCl_3$, 50 °C): δ = 9.67 (s, 2H), 8.34–8.31 (m, 6H), 7.70 (t, *J* = 7.5 Hz, 2H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.24 (d, *J* = 8.2 Hz, 4H), 6.91 (d, *J* = 8.1 Hz, 4H), 6.16 (s, 4H), 3.78 (s, 6H); **^{13}C{^{1}H} NMR** (176 MHz, $CDCl_3$, 50 °C): δ = 159.7 (s, 2C), 138.3 (s, 2C), 127.3 (d, 4C), 126.0 (d, 2C), 123.8 (d, 2C), 122.3 (d, 2C), 117.9 (s, 2C), 115.6 (s, 2C), 115.1 (d, 4C), 99.7 (d, 2C), 55.5 (q, 2C), 49.7 (t, 2C); **HR-MS** (EI+): *m/z* calculated for $[C_{40}H_{30}N_4O_2]^+$, $[M]^+$: 598.2363, found: 598.2347; **IR** (ATR): ν [cm^{-1}] = 3063, 2925, 2853, 1612, 1587, 1560, 1510, 1461, 1442, 1385, 1354, 1328, 1293, 1280, 1241, 1176, 1147, 1119, 1074, 1033, 932, 870, 807, 756, 674, 632; **UV-Vis** (DCM): λ_{max} [nm] = 264, 313, 321, 348, 371, 385; **fluorescence** (DCM): λ_{ex} [nm] = 350, λ_{max} [nm] = 390, 414, 438, 466; **quantum yield** (DCM): Φ = 17%.

Not all carbon peaks could be determined in ^{13}C{^{1}H} NMR due to low solubility.

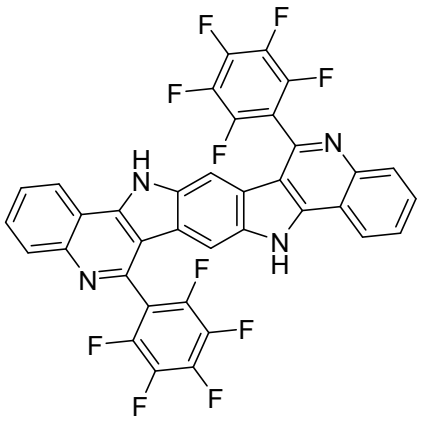
8a



7a (28.5 mg, 38.0 µmol) and $AlCl_3$ (60.7 mg, 455 µmol) were added to a flame-dried Schlenk flask containing anhydrous toluene (3 mL) under an atmosphere of argon and the mixture was stirred at 80 °C for 16 h. The solvent was removed under reduced pressure and the residue was washed subsequently with a diluted solution of KOH in water, water, methanol, DCM and pentane. The product was obtained as a pale yellow solid (15.9 mg, 31.1 µmol, 82%).

Mp: >300 °C; **R_f**: 0.67 (silica gel, EA); **^{1}H NMR** (600 MHz, DMSO-d_6): δ = 12.73 (br, 2H), 8.54 (d, *J* = 8.0 Hz, 2H), 8.13 (d, *J* = 8.2 Hz, 2H), 7.93–7.91 (m, 4H), 7.79–7.72 (m, 10H), 7.69 (t, *J* = 7.3 Hz, 2H); **^{13}C{^{1}H} NMR** (151 MHz, DMSO-d_6): δ = 155.4 (s, 2C), 145.1 (s, 2C), 142.4 (s, 2C), 141.0 (s, 2C), 135.1 (s, 2C), 129.3 (d, 2C), 129.0 (d, 2C), 128.9 (d, 4C), 128.6 (d, 4C), 128.6 (d, 2C), 125.5 (d, 2C), 122.0 (d, 2C), 121.3 (s, 2C), 116.1 (s, 2C), 111.6 (s, 2C), 102.6 (d, 2C); **HR-MS** (EI+): *m/z* calculated for $[C_{36}H_{22}N_4]^+$, $[M]^+$: 510.18390, found: 510.18172; **IR** (ATR): ν [cm^{-1}] = 3174, 3130, 3078, 2908, 2839, 2771, 2255, 2242, 2124, 1954, 1625, 1565, 1531, 1510, 1492, 1444, 1405, 1358, 1302, 1258, 1223, 1192, 1171, 1150, 1109, 1071, 1046, 1020, 995, 949, 909, 851, 820, 764, 736, 698, 660, 626; **UV-Vis** (DCM): λ_{max} [nm] = 262, 318, 328, 364; (THF): λ_{max} [nm] = 262, 323, 369; (DMSO): λ_{max} [nm] = 260, 327, 338, 370; **fluorescence** (DCM): λ_{ex} [nm] = 350, λ_{max} [nm] = 395, 413; (THF): λ_{ex} [nm] = 350, λ_{max} [nm] = 402, 419, 442; (DMSO): λ_{ex} [nm] = 350, λ_{max} [nm] = 407, 429; **quantum yield** (DCM): Φ = 10%; (THF): Φ = 15%; (DMSO): Φ = 7%.

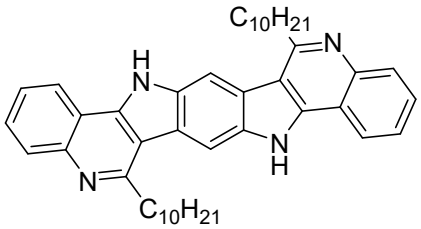
8b



7b (13.0 mg, 14.0 µmol) and $AlCl_3$ (22.4 mg, 168 µmol) were added to a flame-dried Schlenk flask containing anhydrous toluene (3 mL) under an atmosphere of argon and the mixture was stirred at 80 °C for 16 h. TLC did not show full conversion, therefore additional $AlCl_3$ (44.7 mg, 335 µmol) was added and the mixture was stirred at 110 °C for 16 h. A saturated aqueous solution of $NaHCO_3$ was added and the mixture was extracted with DCM. The combined organic layers were washed with water and brine, dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash column chromatography (silica gel, PE:EA = 10:1 to 1:1 to DCM:MeOH = 9:1 to 3:1) and further washed with EA/pentane and pentane. The product was obtained as a pale yellow solid (6.40 mg, 9.27 µmol, 66%).

Mp: >300 °C; $\mathbf{R_f}$: 0.37 (silica gel, DCM:MeOH = 9:1); **^{1}H NMR** (301 MHz, DMSO-d_6): δ = 13.06 (s, 2H), 8.66–8.63 (m, 2H), 8.21–8.18 (m, 2H), 7.89–7.80 (m, 4H), 7.61 (s, 2H); **^{13}C{^{1}H} NMR** (176 MHz, DMSO-d_6, 80 °C): δ = 160.0 (s, 2C), 144.8 (s, 2C), 144.0 (s, J = 248 Hz, 4CF), 142.1 (s, J = 224 Hz, 2CF),142.1 (s, 2C), 140.3 (s, 2C), 137.4 (s, J = 250 Hz, 4CF), 135.3 (s, 2C), 129.1 (d, 2C), 128.6 (d, 2C), 126.3 (d, 2C), 121.9 (d, 2C), 120.2 (s, 2C), 116.2 (s, 2C), 112.8 (s, 2C), 101.2 (d, 2C); **^{19}F{^{1}H} NMR** (283 MHz; DMSO-d_6): δ = −142.4 (dd, J = 24.5 Hz, J = 7.9 Hz, 4F), −153.5 (t, J = 22.2 Hz, 2F), −160.6–(−160.8) (m, 4F); **HR-MS** (MALDI+): *m/z* calculated for $[C_{36}H_{12}F_{10}N_4]^+$, $[M]^+$: 690.0897, found: 690.0879; **IR** (ATR): ν [cm^{-1}] = 3190, 3151, 2913, 2845, 2779, 2248, 2126, 1655, 1570, 1493, 1450, 1408, 1357, 1315, 1286, 1261, 1207, 1191, 1156, 1109, 1024, 986, 923, 878, 842, 822, 759, 726, 676, 632; **UV-Vis** (DCM): λ_{max} [nm] = 258, 314, 327, 346, 364 ; (THF): λ_{max} [nm] = 255, 317, 330, 369; **fluorescence** (DCM): λ_{ex} [nm] = 350, λ_{max} [nm] = 393, 409; (THF): λ_{ex} [nm] = 350, λ_{max} [nm] = 402, 419; **quantum yield** (DCM): Φ = 18%; (THF): Φ = 22%.

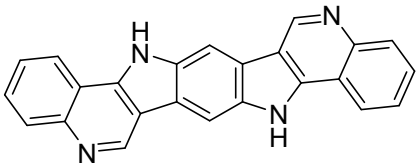
8c



7c (36.0 mg, 40.9 µmol) and $AlCl_3$ (65.5 mg, 491 µmol) were added to a flame-dried Schlenk flask containing anhydrous toluene (5 mL) under an atmosphere of nitrogen and the mixture was stirred at 80 °C for 16 h. A saturated aqueous solution of $NaHCO_3$ was added and the mixture was extracted with a large amount of EA. The combined organic layers were washed with water and brine, dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash column chromatography (silica gel, PE:EA = 1:1 to DCM:MeOH = 9:1 to 3:1) and further washed with EA/pentane and pentane. The product was obtained as a pale yellow solid (19.8 mg, 31.0 µmol, 76%).

Mp: >300 °C; $\mathbf{R_f}$: 0.57 (silica gel, DCM:MeOH = 9:1); **^{1}H NMR** (700 MHz, DMSO-d_6, 120 °C): δ = 12.28 (br, 2H), 8.52–8.51 (m, 2H), 8.43–8.42 (m, 2H), 8.08–8.07 (m, 2H), 7.71–7.70 (m, 2H), 7.63–7.61 (m, 2H), 3.58–3.56 (m, 4H), 2.12 (br, 4H), 1.67 (br, 4H), 1.48 (br, 4H), 1.36–1.25 (m, 20H), 0.84–0.83 (m, 6H); **^{13}C{^{1}H} NMR** (176 MHz, DMSO-d_6, 120 °C): δ = 157.2 (s, 2C), 144.6 (s, 2C), 141.3 (s, 2C), 135.2 (s, 2C), 128.3 (d, 2C), 127.22 (d, 2C), 123.8 (d, 2C), 121.1 (d, 2C), 120.7 (s, 2C), 115.6 (s, 2C), 111.9 (s, 2C), 102.3 (d, 2C), 36.5 (t, 2C), 30.5 (t, 2C), 28.5 (t, 2C), 28.3 (t, 2C), 28.3 (t, 2C), 28.2 (t, 2C), 27.9 (t, 2C), 26.8 (t, 2C), 21.2 (t, 2C), 12.9 (q, 2C); **HR-MS** (ESI+): *m/z* calculated for $[C_{44}H_{55}N_4]^+$, $[M+H]^+$: 639.4421, found: 639.4426; **IR** (ATR): ν [cm^{-1}] = 2922, 2851, 1734, 1568, 1536, 1510, 1456, 1422, 1359, 1298, 1261, 1193, 1093, 1030, 920, 847, 818, 762, 611; **UV-Vis** (DCM): λ_{max} [nm] = 260, 306, 314, 340, 358, 373; (THF): λ_{max} [nm] = 262, 308, 316, 342, 352, 359, 378; **fluorescence** (DCM): λ_{ex} [nm] = 350, λ_{max} [nm] = 379, 400, 420, 450; (THF): λ_{ex} [nm] = 350, λ_{max} [nm] = 384, 406, 426, 456; **quantum yield** (DCM): Φ = 24%; (THF): Φ = 52%.

8d



7d (12.7 mg, 21.2 µmol) and $AlCl_3$ (33.9 mg, 255 µmol) were added to a flame-dried Schlenk flask containing anhydrous toluene (2 mL) under an atmosphere of argon and the mixture was stirred at 80 °C for 16 h. A saturated aqueous solution of $NaHCO_3$ was added and the mixture was extracted with a large amount of EA. The combined organic layers were washed with water and brine, dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash column chromatography (silica gel, PE:EA = 1:1 to EA to DCM:MeOH = 9:1 to 3:1) and further washed with EA/pentane and pentane. The product was obtained as a pale yellow solid (5.10 mg, 14.2 µmol, 67%).

Mp: >300 °C; **R_f**: 0.43 (silica gel, DCM:MeOH = 9:1); **^{1}H NMR** (700 MHz, DMSO-d_6, 100 °C): δ = 12.88 (br, 2H), 9.68 (s, 2H), 8.74 (d, *J* = 8.0 Hz, 2H), 8.54 (s, 2H), 8.15 (d, *J* = 8.3 Hz, 2H), 7.73 (t, *J* = 7.4 Hz, 2H), 7.66 (t, *J* = 7.4 Hz, 2H); **^{13}C{^{1}H} NMR** (176 MHz, DMSO-d_6, 100 °C): δ = 145.4 (s, 2C), 144.0 (d, 2C), 140.9 (s, 2C), 135.2 (s, 2C), 128.9 (d, 2C), 127.2 (d, 2C), 124.6 (d, 2C), 122.2 (d, 2C), 121.4 (s, 2C), 116.7 (s, 2C), 113.9 (s, 2C), 100.8 (d, 2C); **HR-MS** (EI+): *m/z* calculated for $[C_{24}H_{14}N_4]^+$, $[M]^+$: 358.12130, found: 358.12100; **IR** (ATR): ν [cm^{-1}] = 3371, 2924, 2835, 1598, 1543, 1514, 1424, 1262, 1219, 1187, 1111, 1028, 768, 662; **UV-Vis** (DCM): λ_{max} [nm] = 258, 310, 317, 338, 359, 370; (THF): λ_{max} [nm] = 258, 311, 320, 327, 341, 363, 374; **fluorescence** (DCM): λ_{ex} [nm] = 350, λ_{max} [nm] = 382, 402, 422, 452; (THF): λ_{ex} [nm] = 350, λ_{max} [nm] = 384, 404, 427, 454; **quantum yield** (DCM): Φ = 9%; (THF): Φ = 30%.

2 NMR Spectra

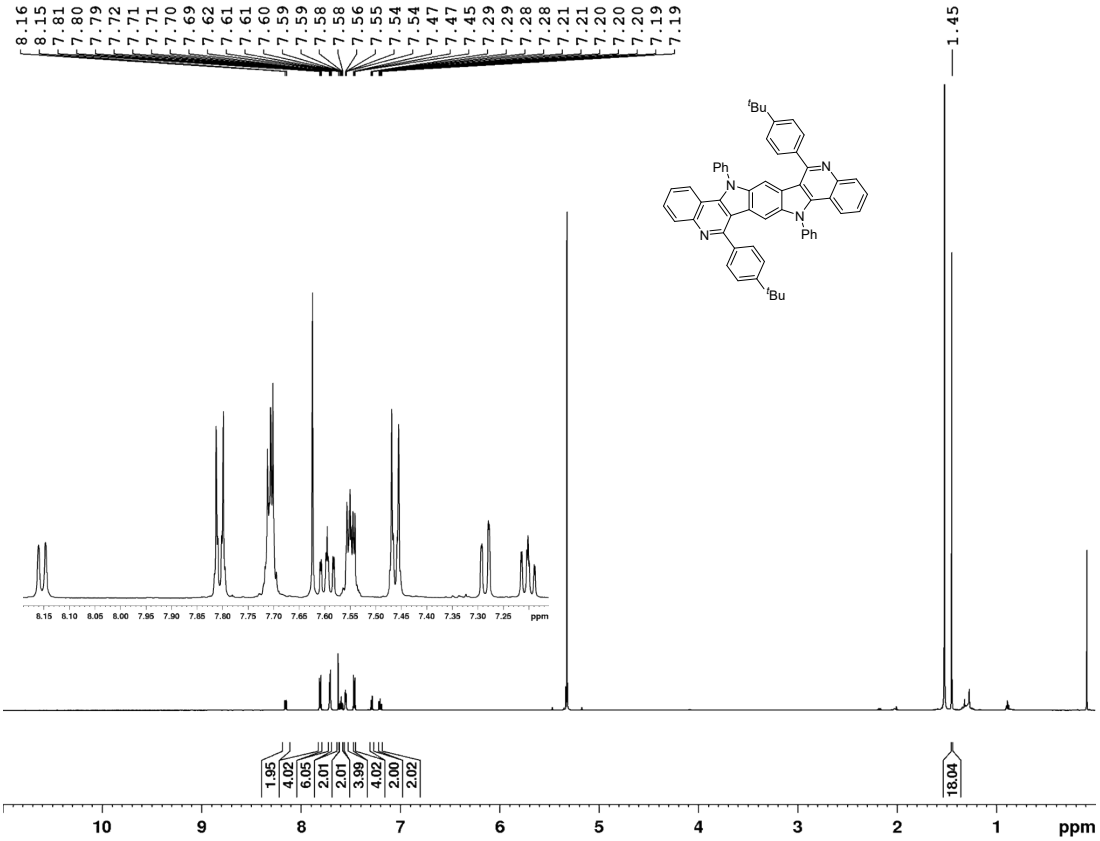


Figure S1. ^{1}H NMR spectrum (600 MHz, CD_2Cl_2, 32 °C) of **2a**.

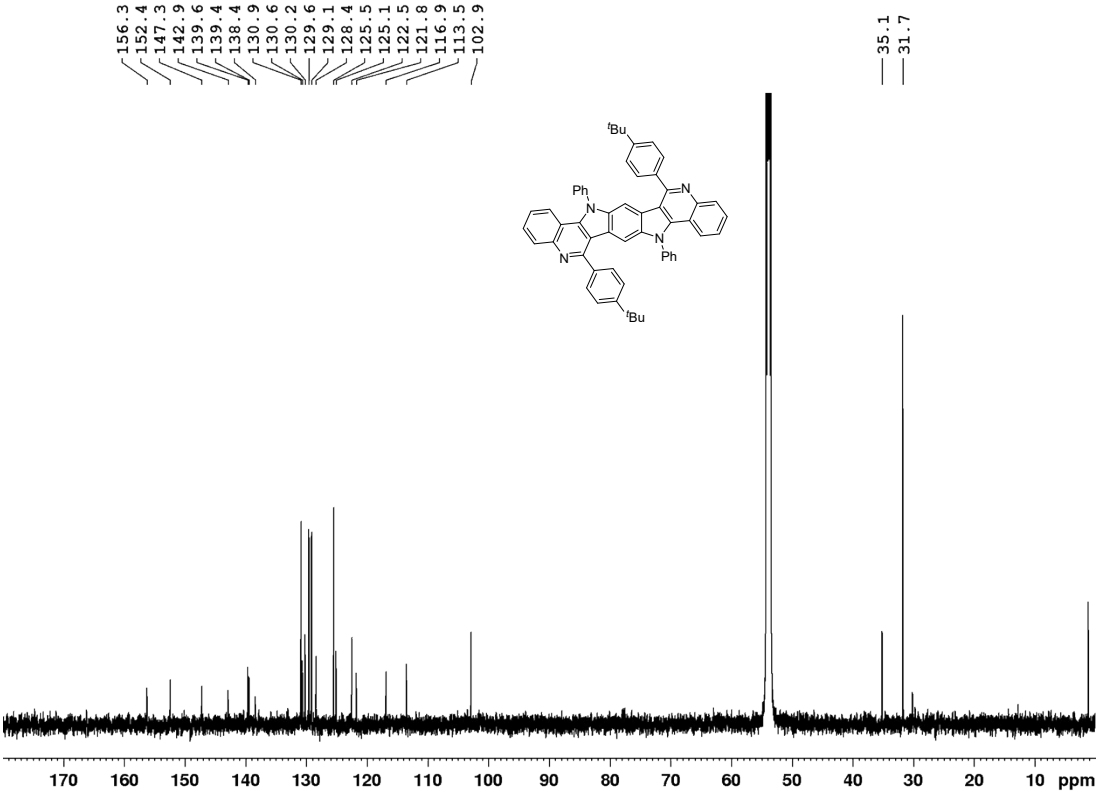


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, CD_2Cl_2, 32 °C) of **2a**.

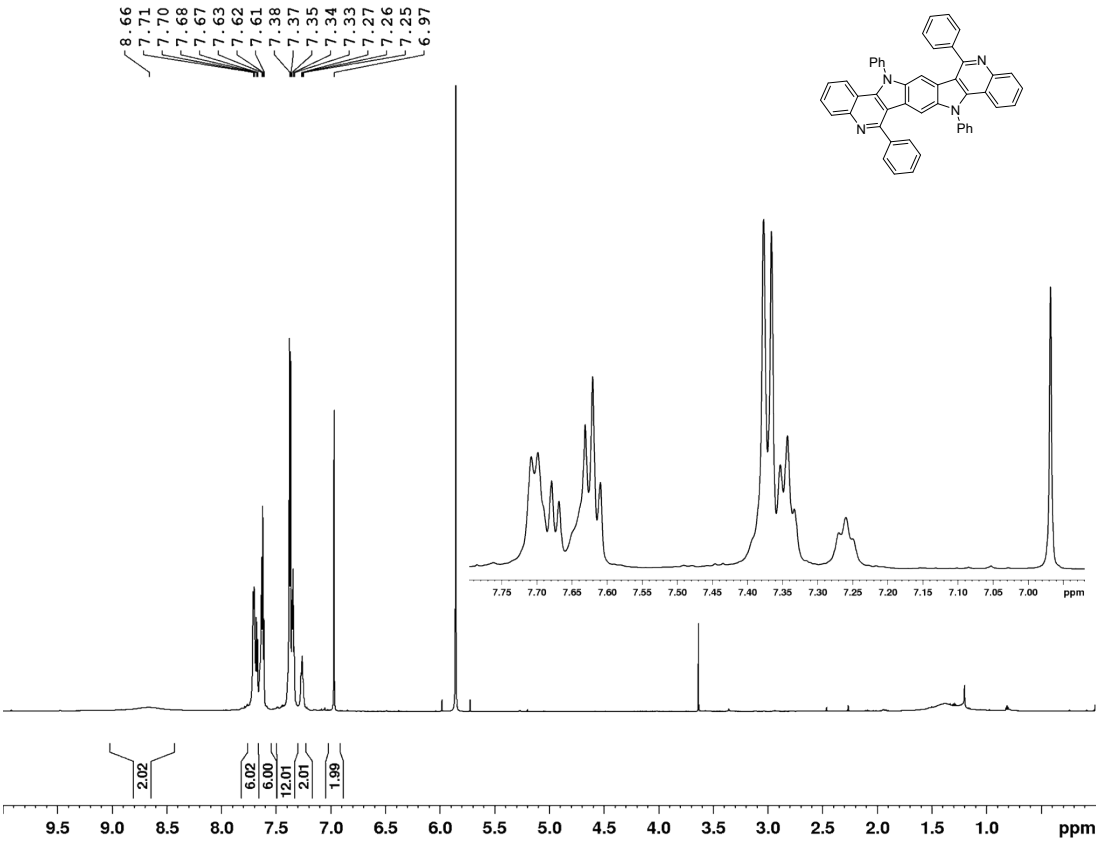


Figure S3. ^{1}H NMR spectrum (700 MHz, TCE-d_2, 100 °C) of **2b**.

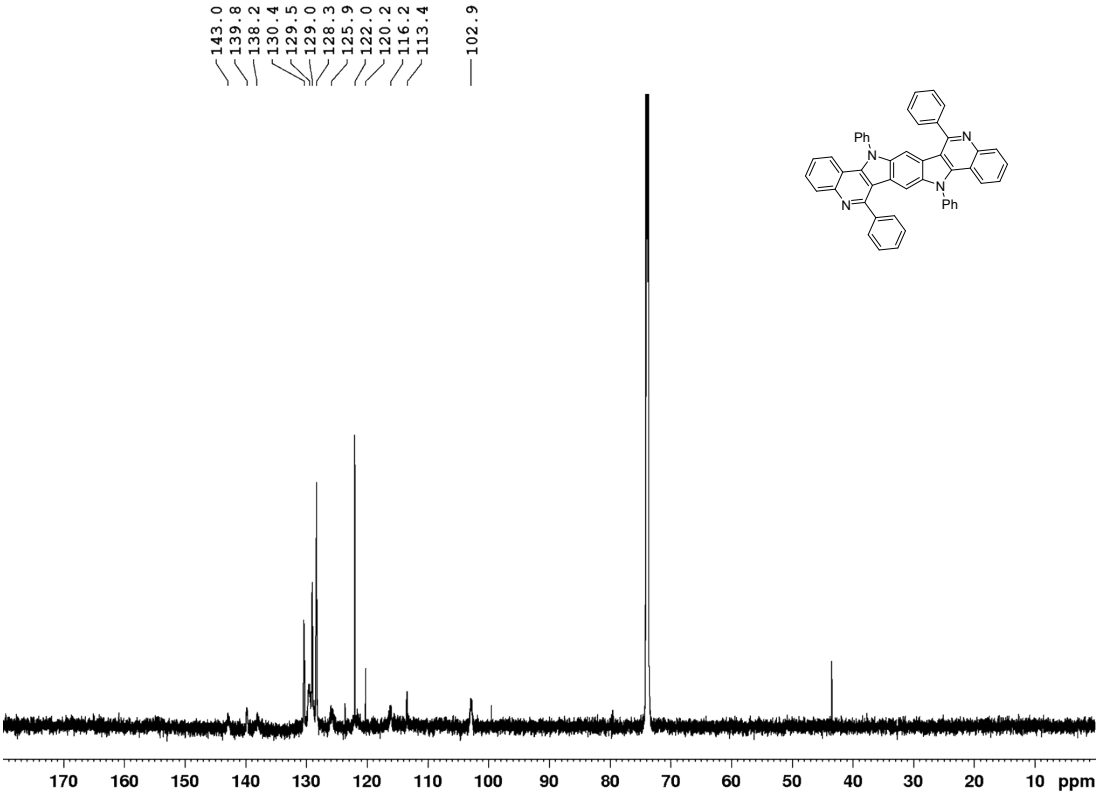


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, TCE-d_2, 100 °C) of **2b**.

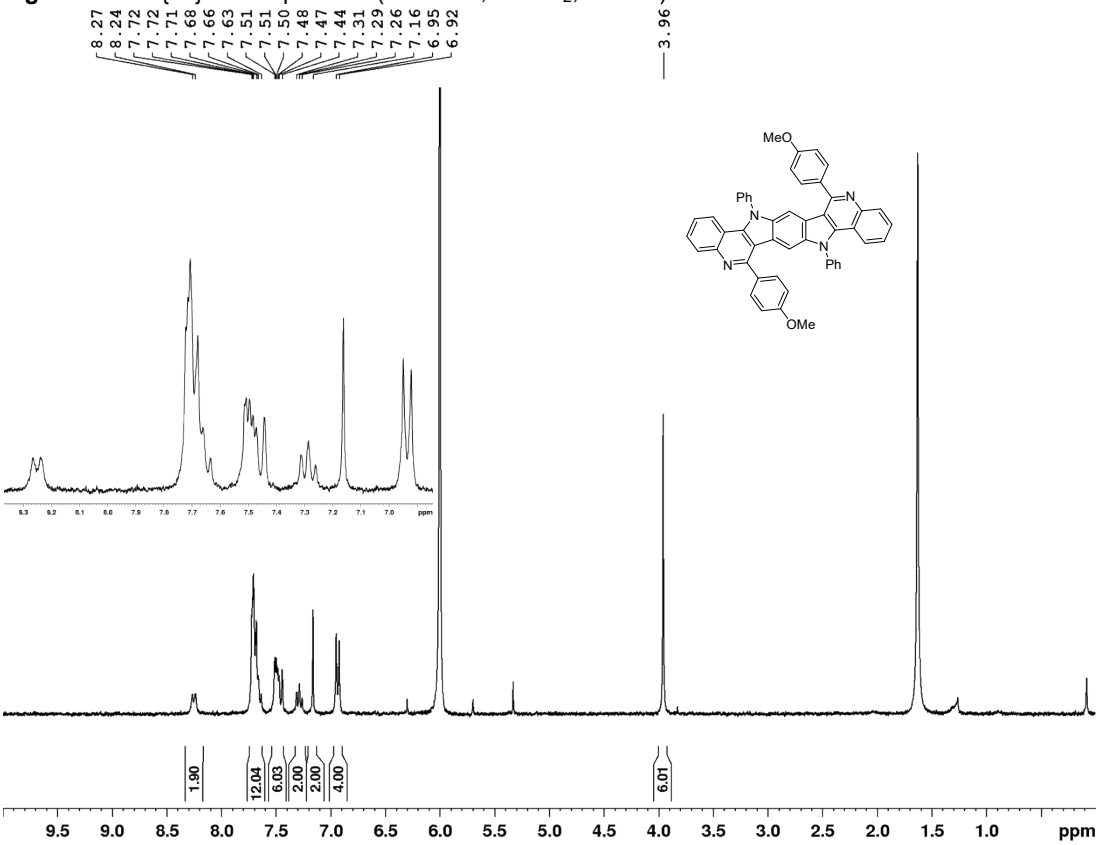


Figure S5. ^{1}H NMR spectrum (301 MHz, TCE-d_2) of **2c**.

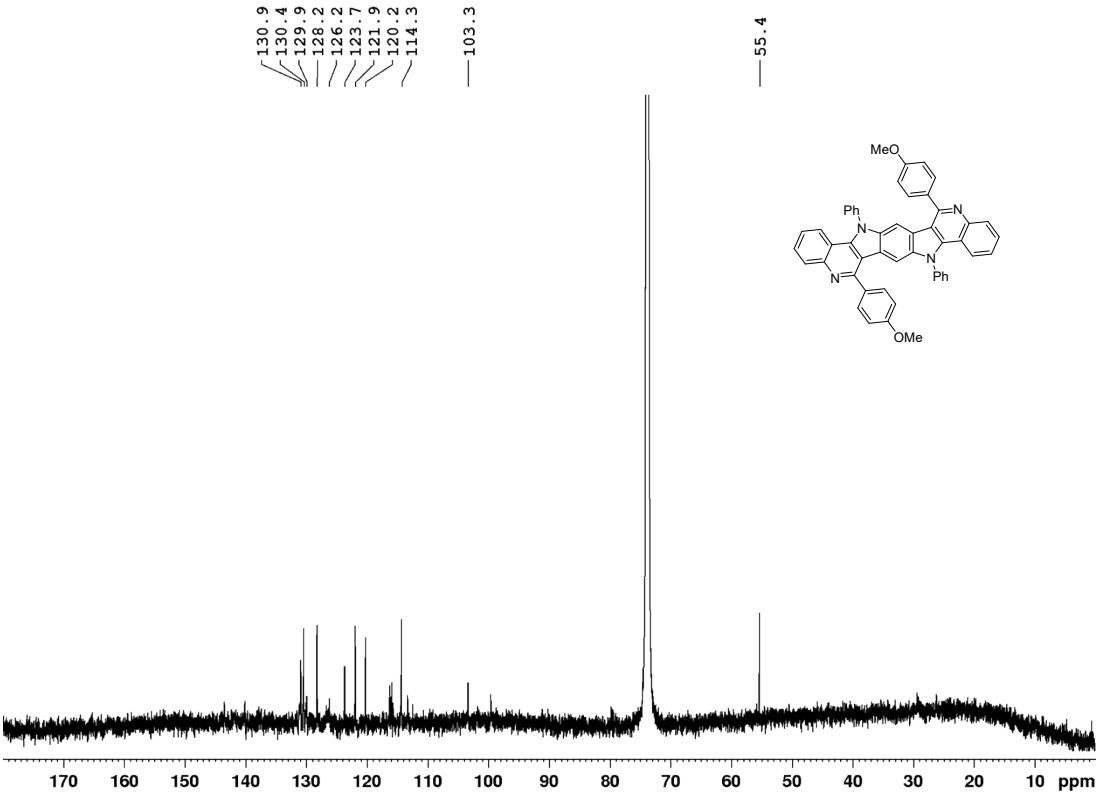


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, TCE-d_2, 140 °C) of **2c**.

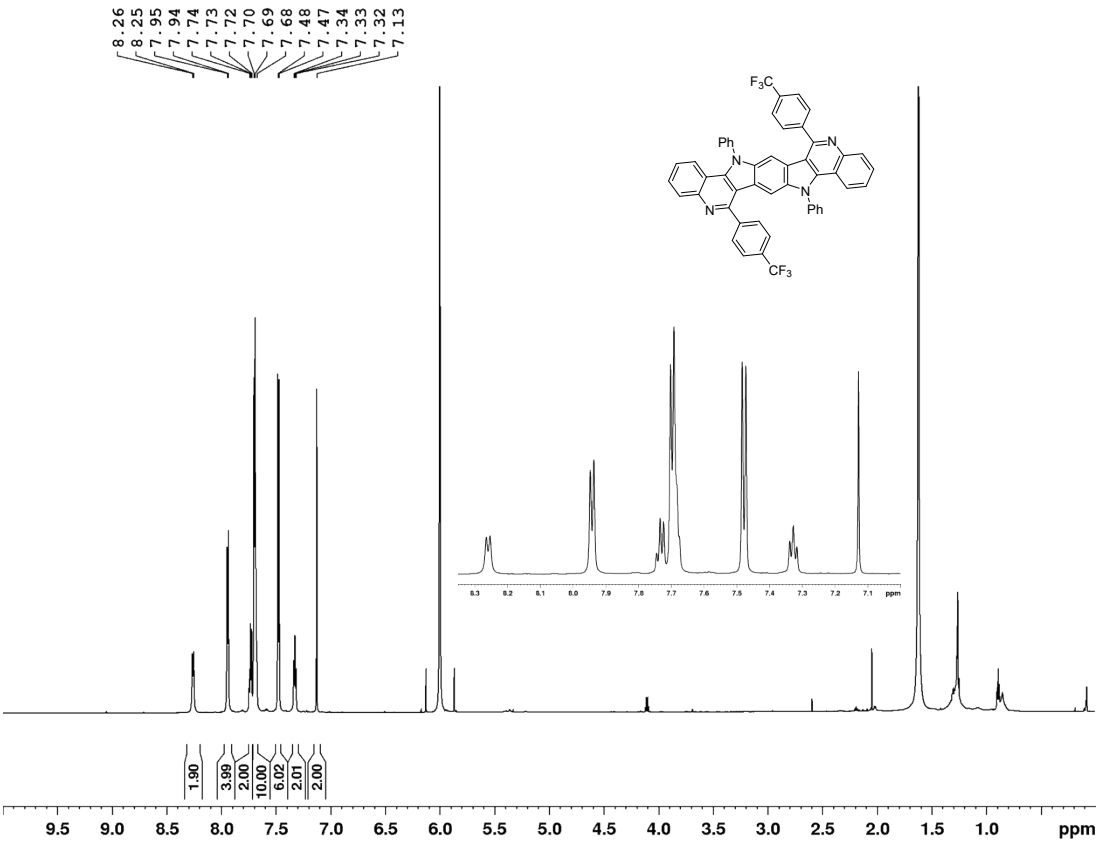


Figure S7. ^{1}H NMR spectrum (700 MHz, TCE-d_2) of **2d**.

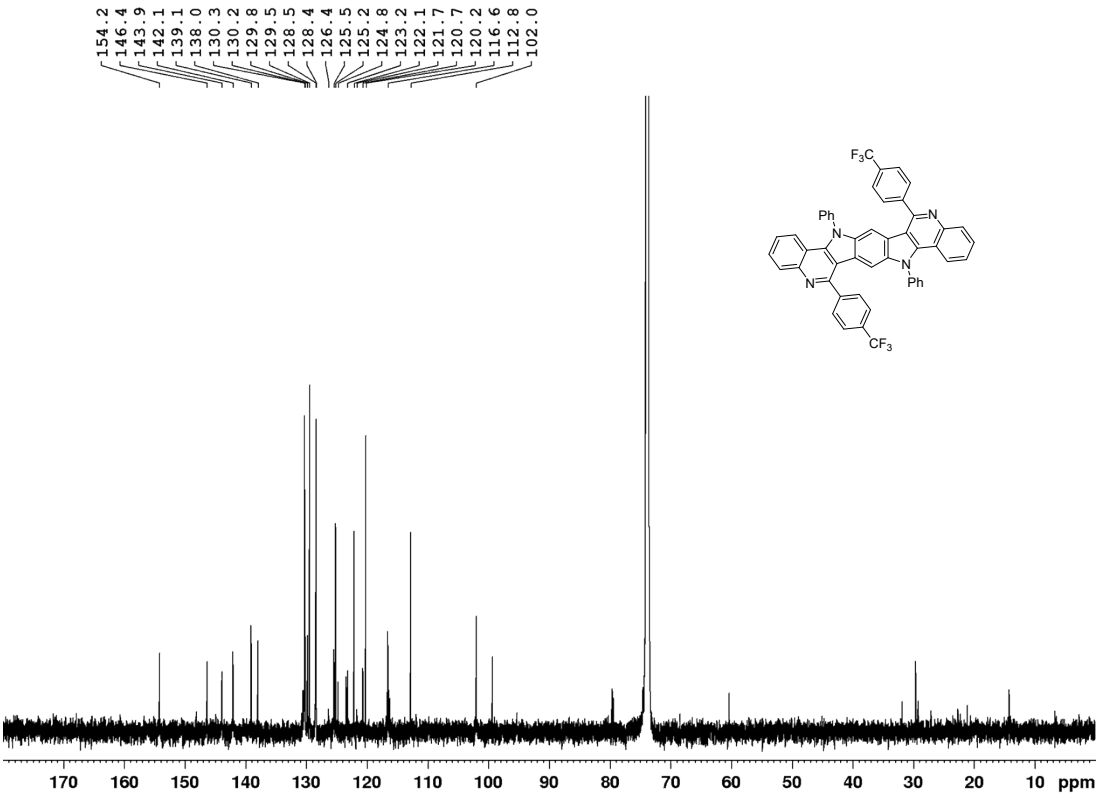


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, TCE-d_2) of **2d**.

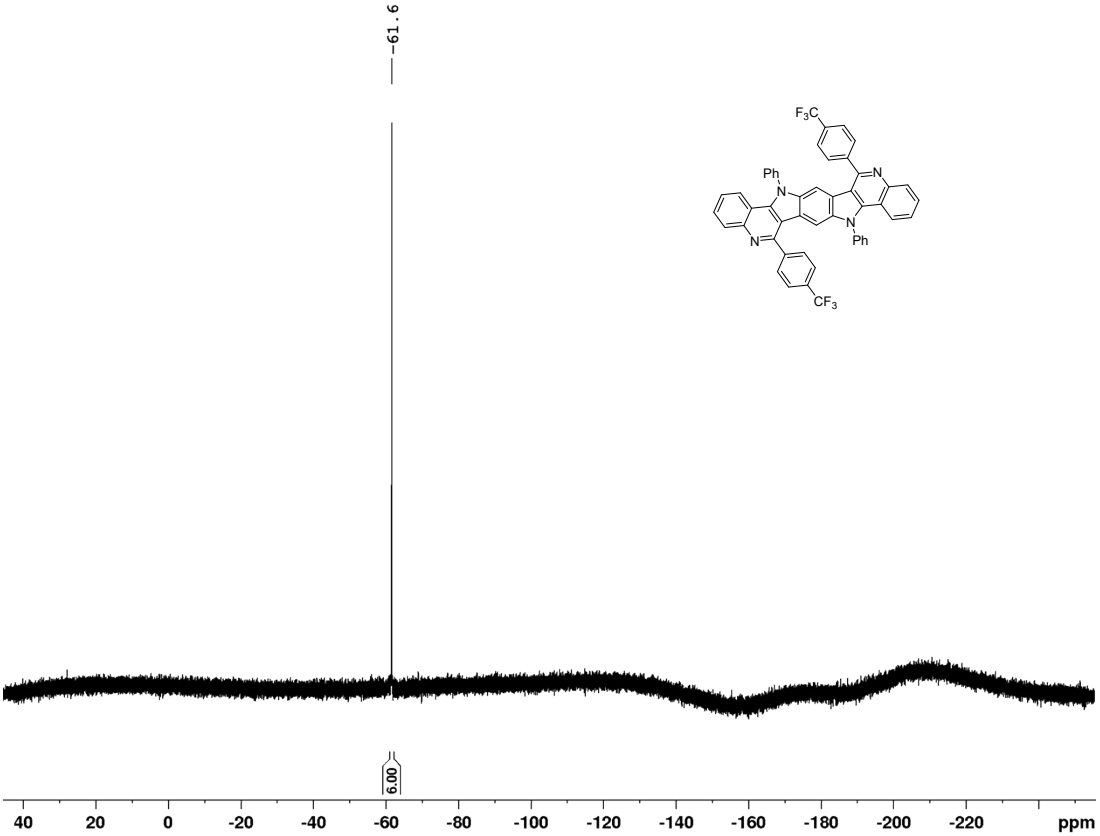


Figure S9. $^{19}F\{^{1}H\}$ spectrum (283 MHz, TCE-d_2) of **2d**.

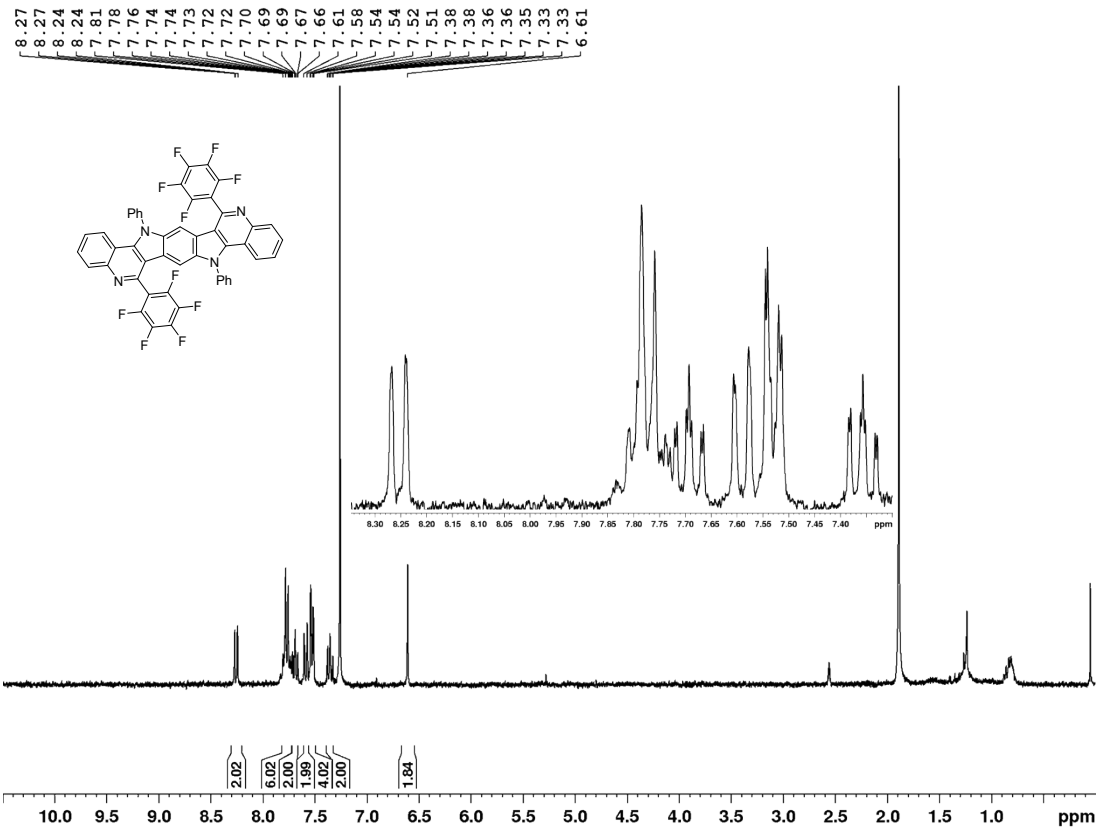


Figure S10. ^{1}H NMR spectrum (301 MHz, $CDCl_3$) of **2e**.

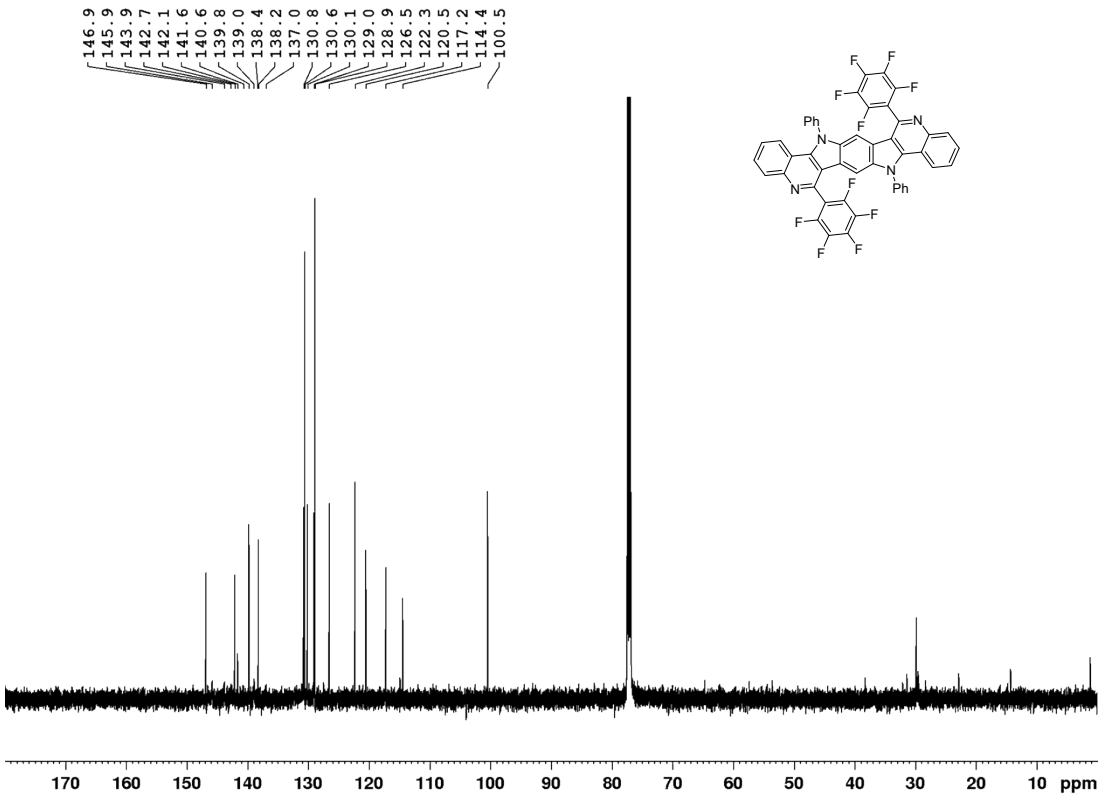


Figure S11. $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, $CDCl_3$) of **2e**.

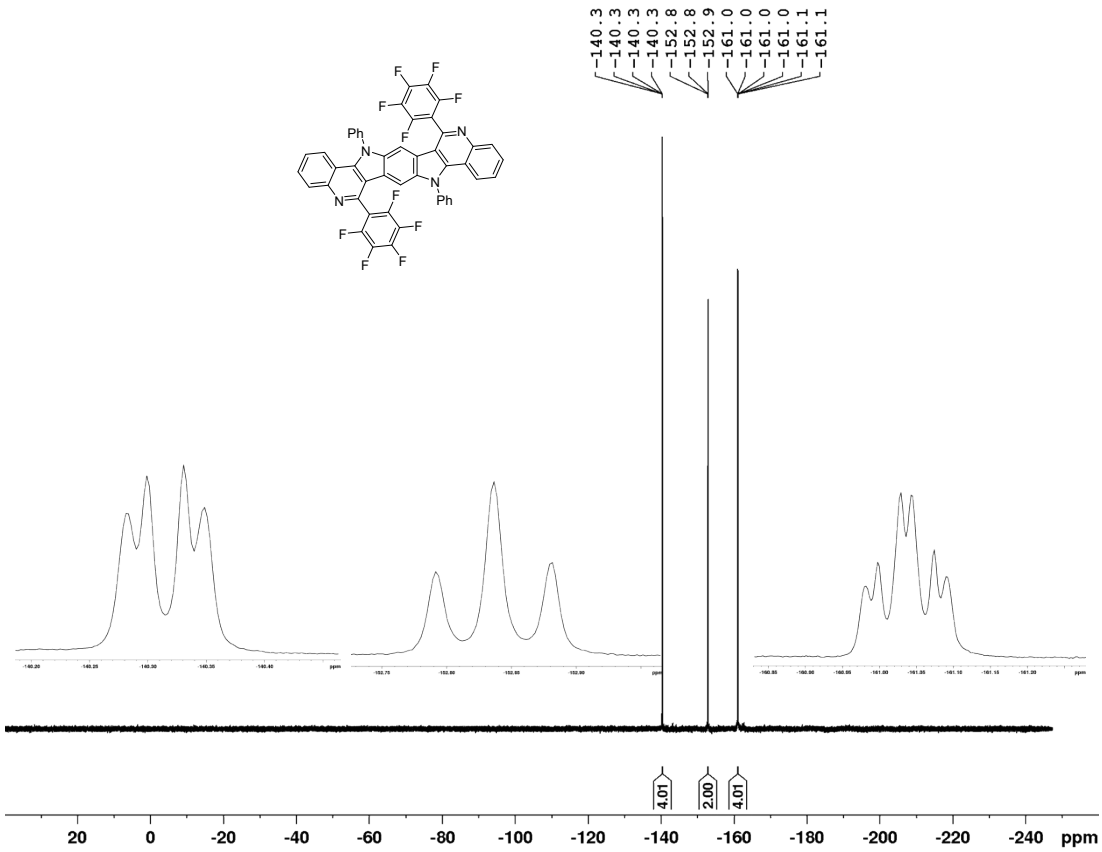


Figure S12. $^{19}F\{^{1}H\}$ spectrum (471 MHz, $CDCl_3$) of **2e**.

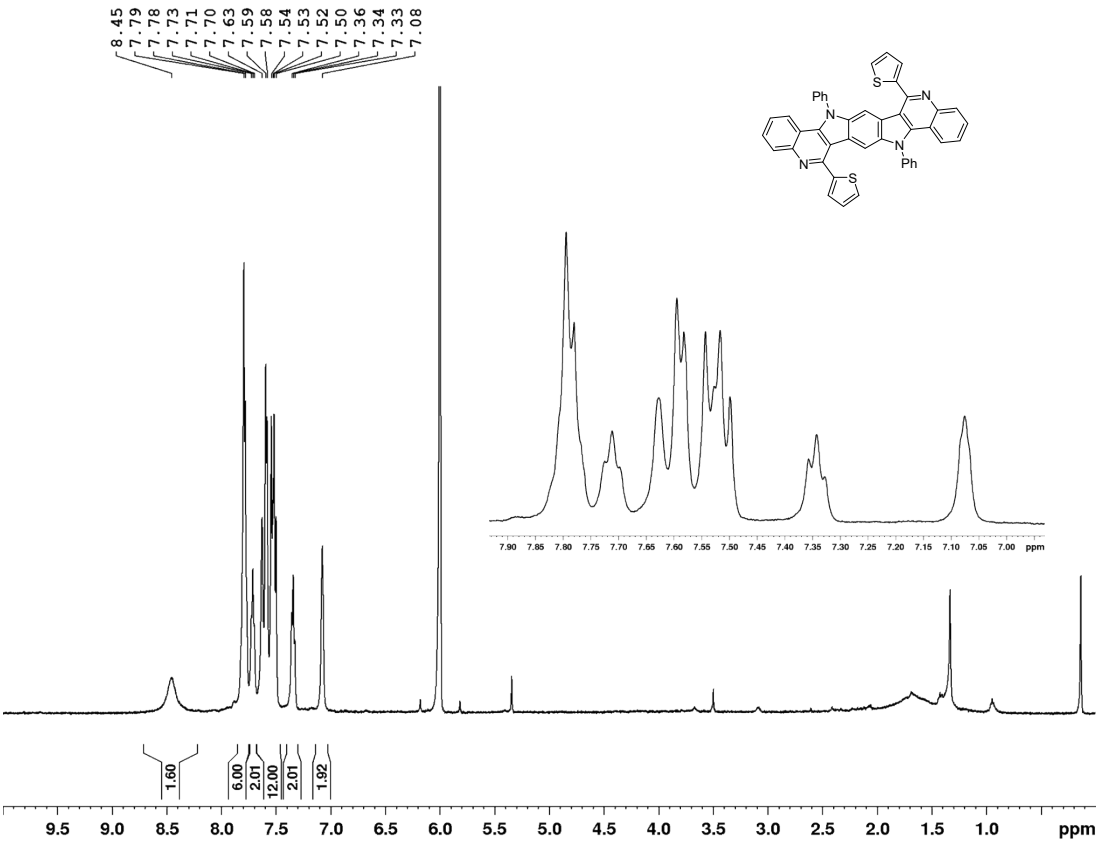


Figure S13. ^{1}H NMR spectrum (500 MHz, TCE-d_2, 80 °C) of **2f**.

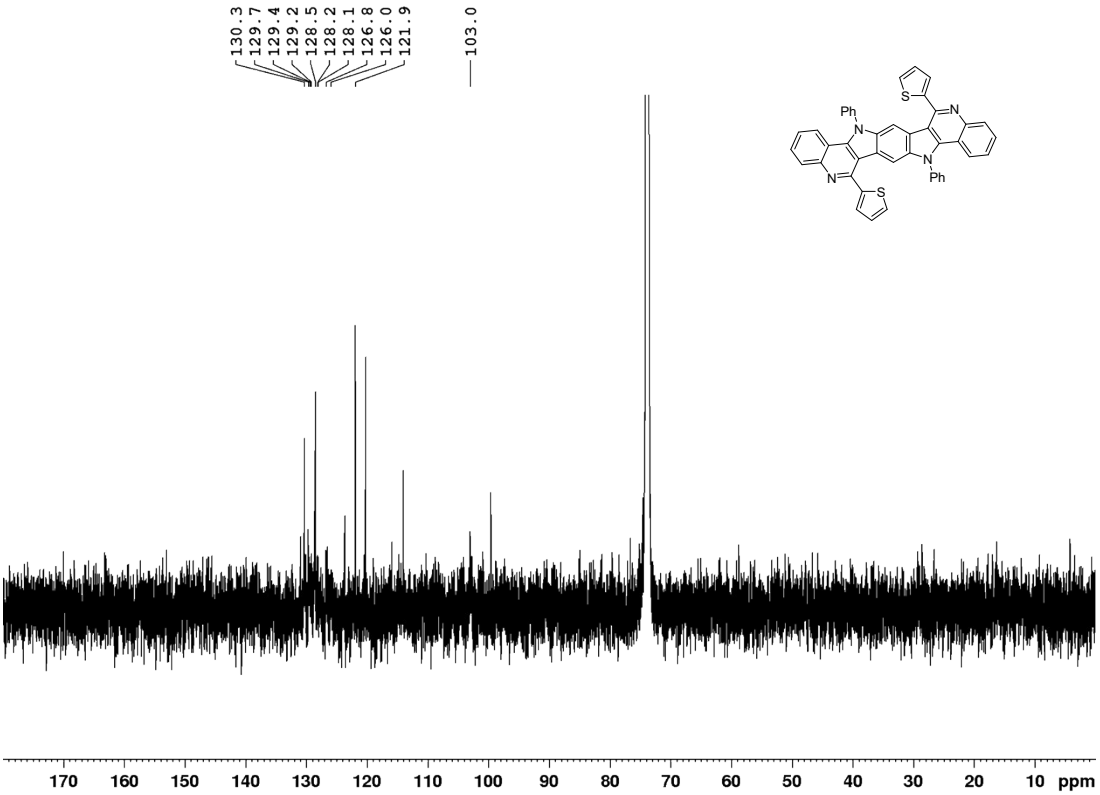


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, TCE-d_2, 140 °C) of **2f**.

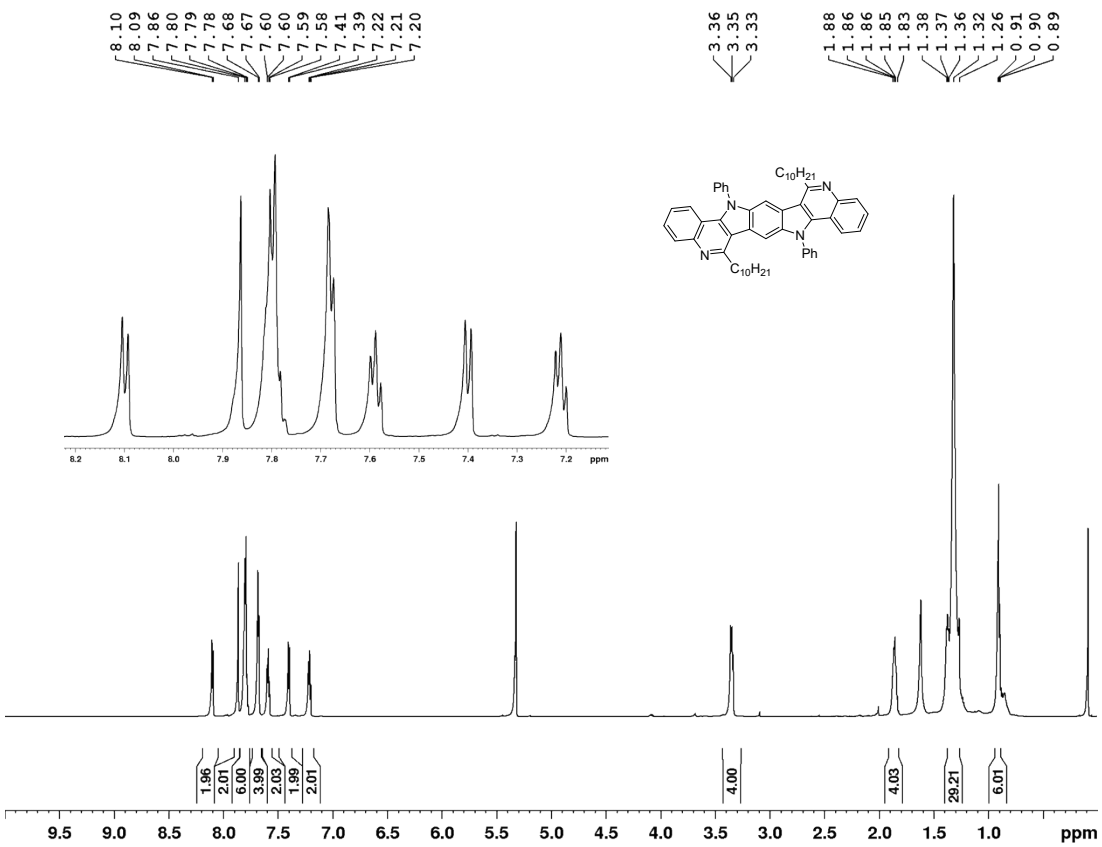


Figure S15. ^{1}H NMR spectrum (700 MHz, CD_2Cl_2) of **2g**.

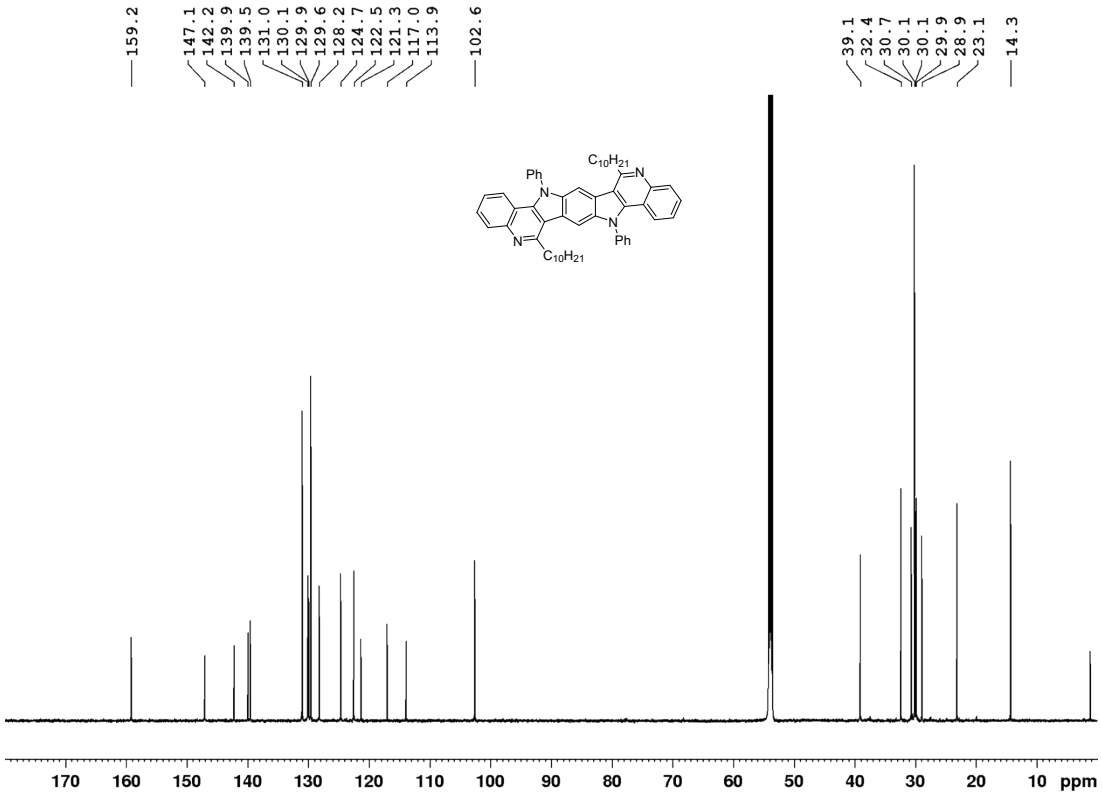


Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, CD_2Cl_2) of **2g**.

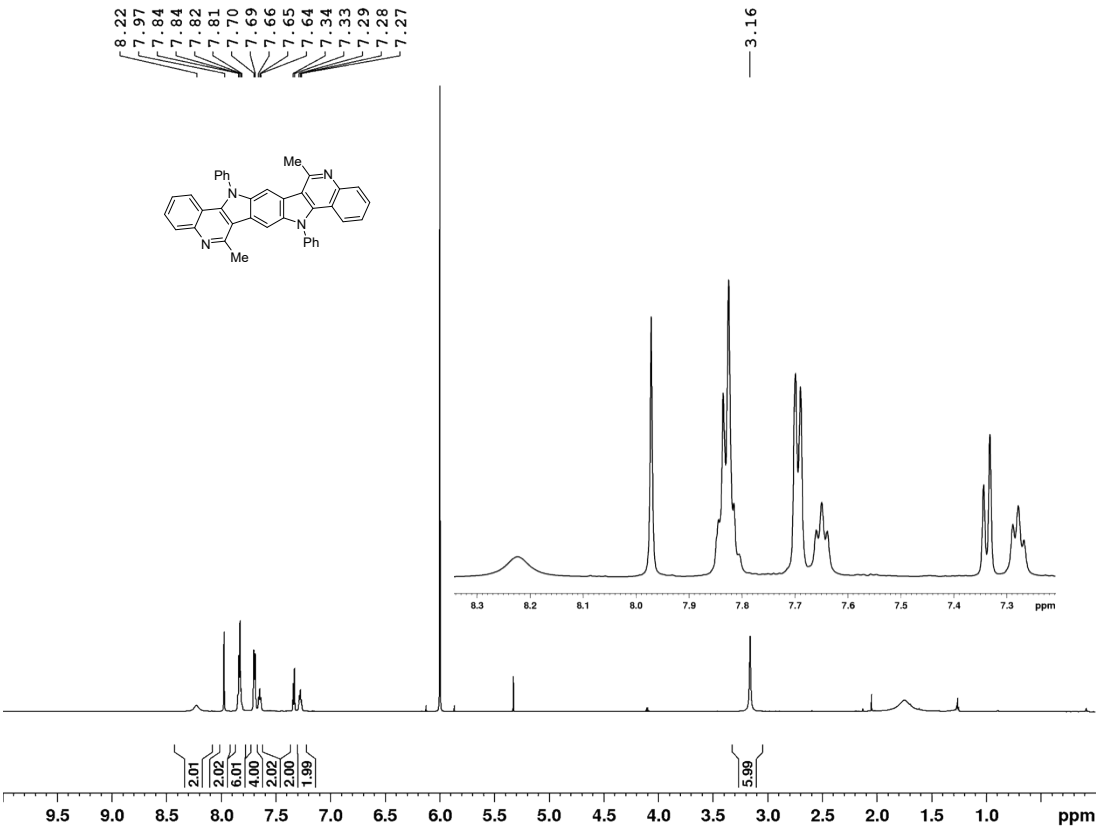


Figure S17. ^{1}H NMR spectrum (700 MHz, TCE-d_2) of **2h**.

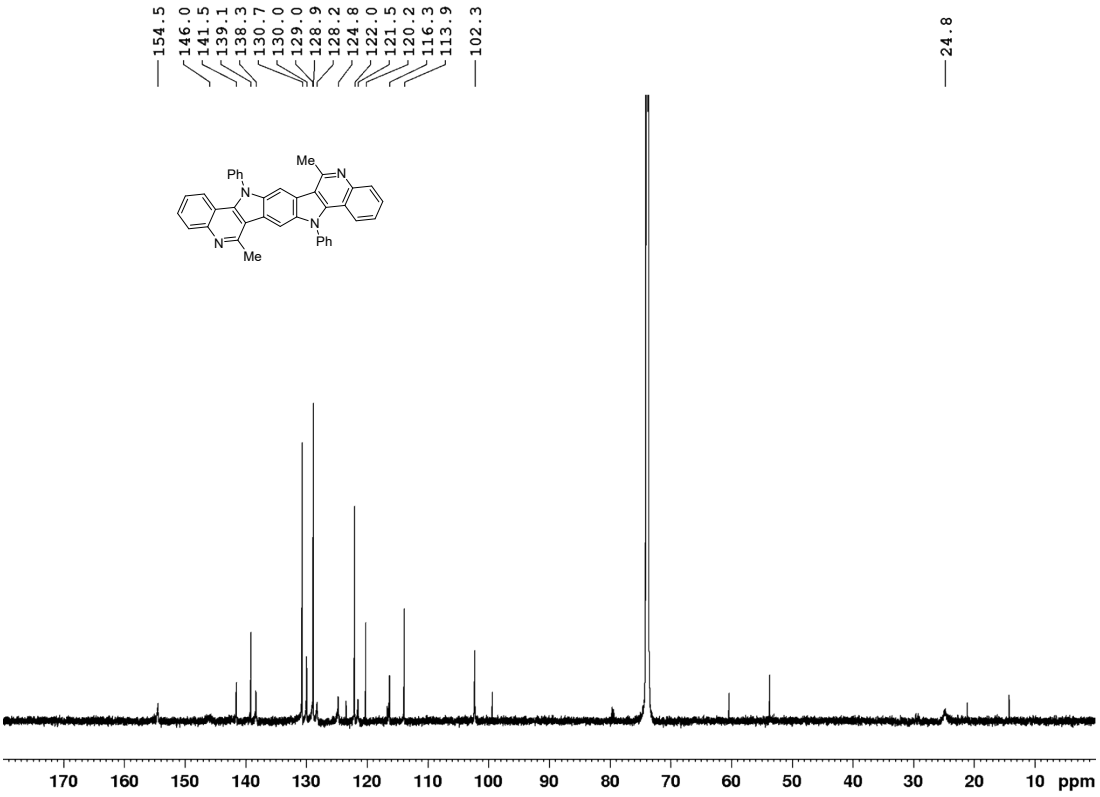


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, TCE-d_2) of **2h**.

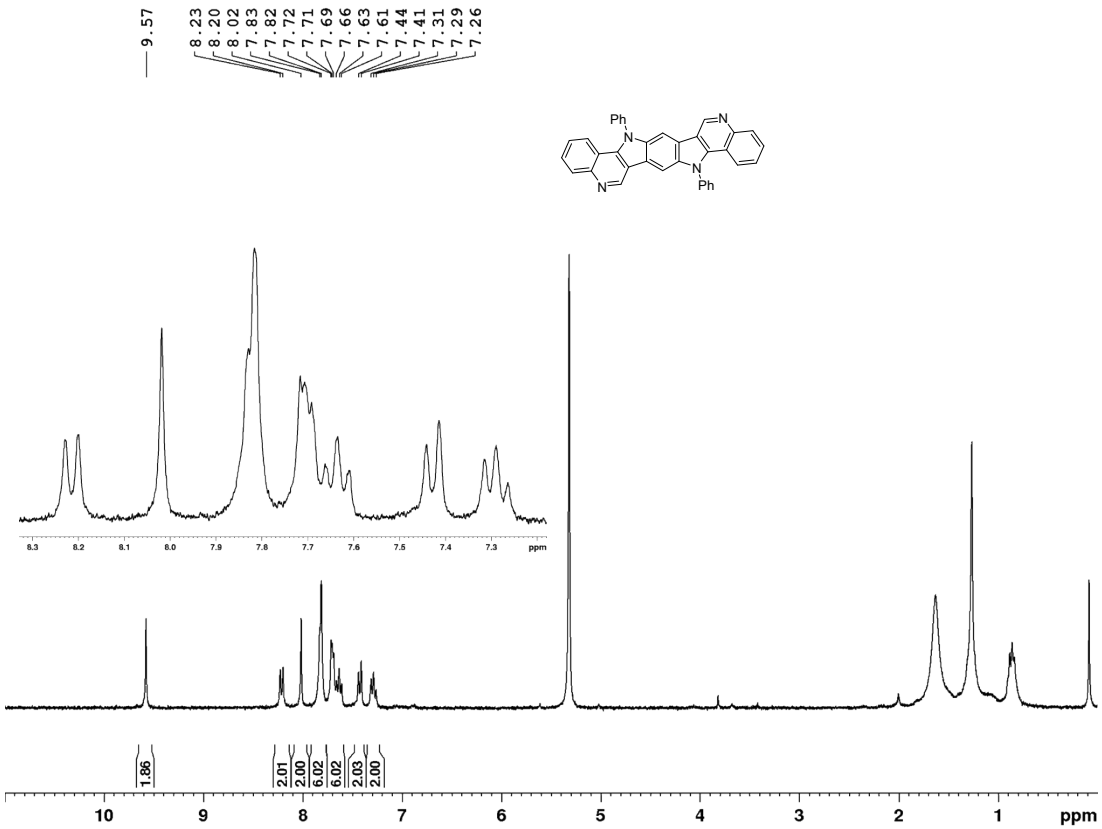


Figure S19. ^{1}H NMR spectrum (301 MHz, CD_2Cl_2) of **2i**.

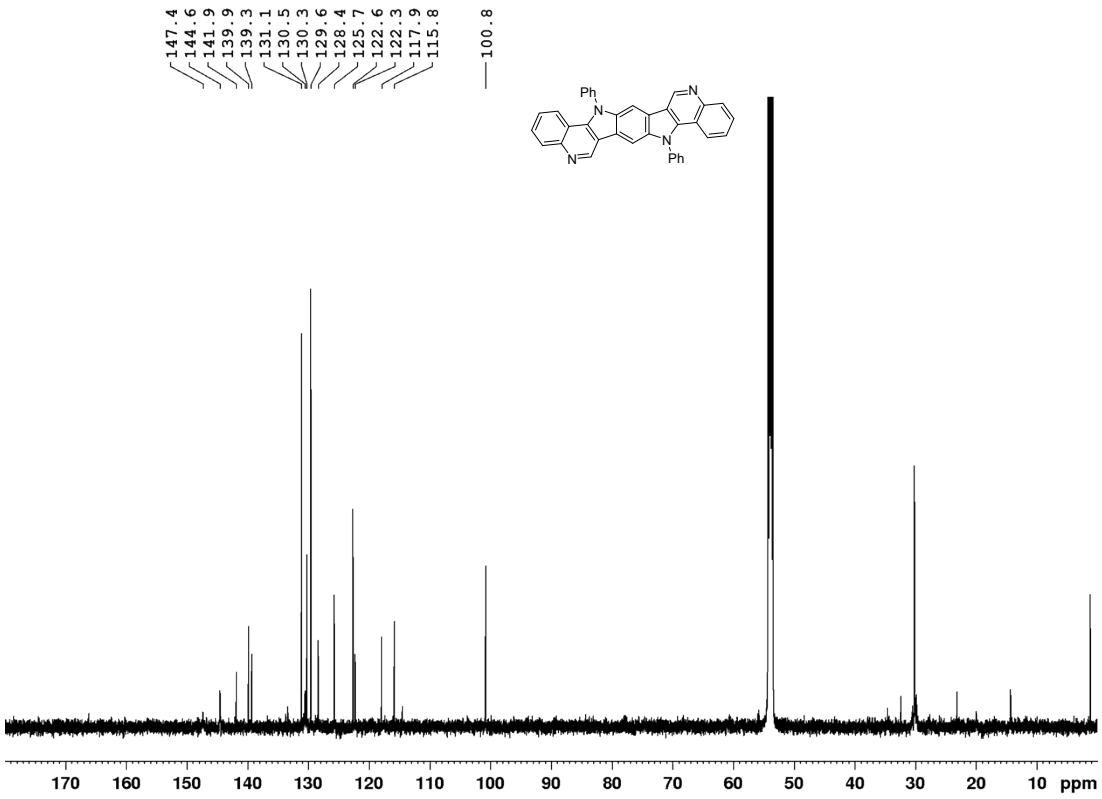


Figure S20. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, CD_2Cl_2, 32 °C) of **2i**.

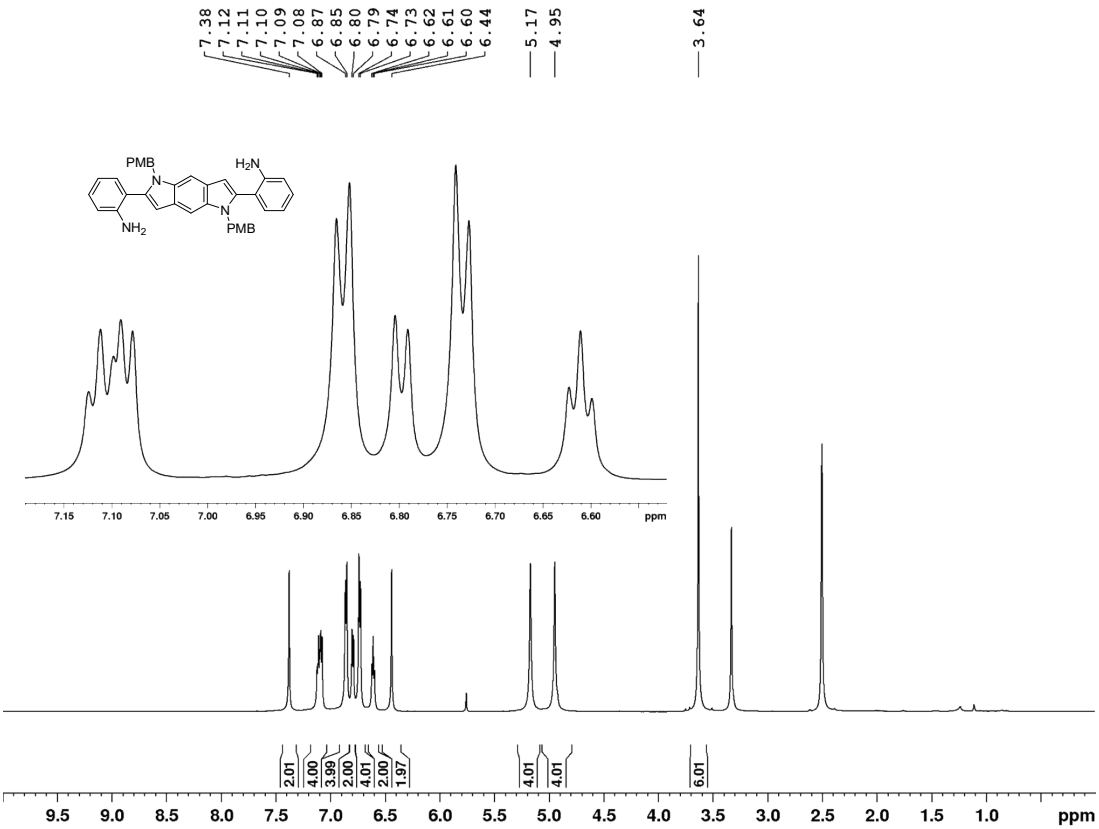


Figure S21. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of **5**.

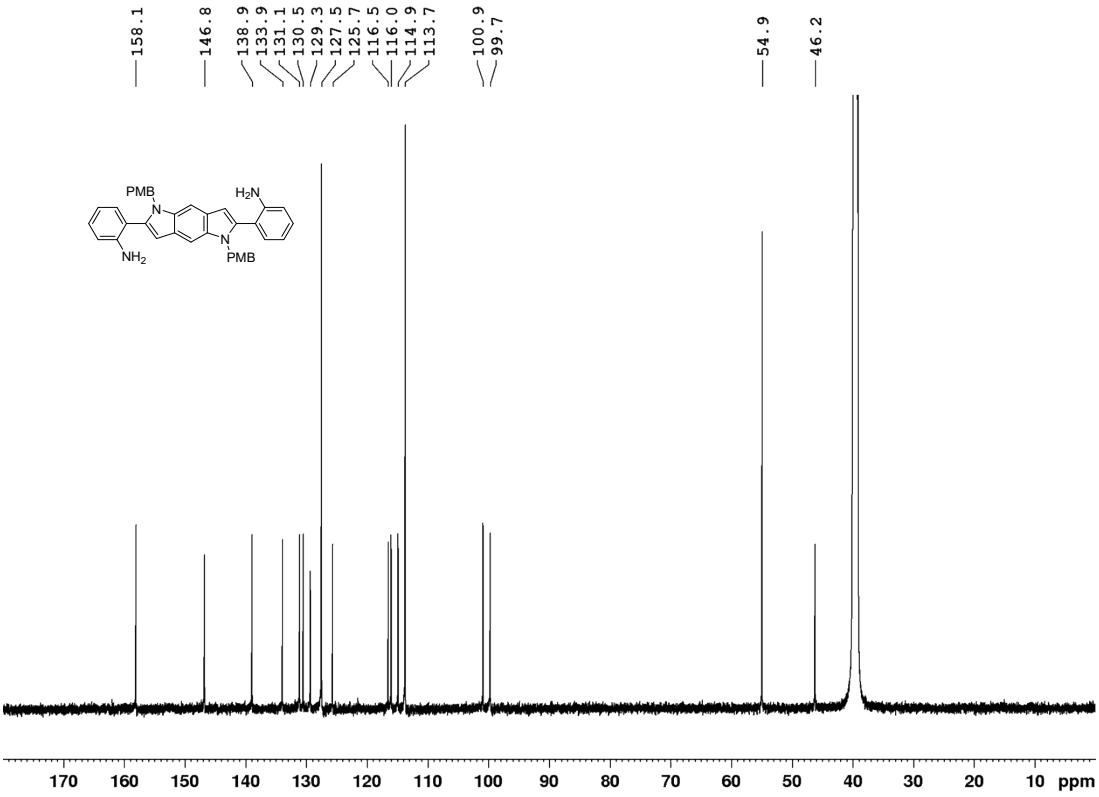


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, DMSO-d_6) of **5**.

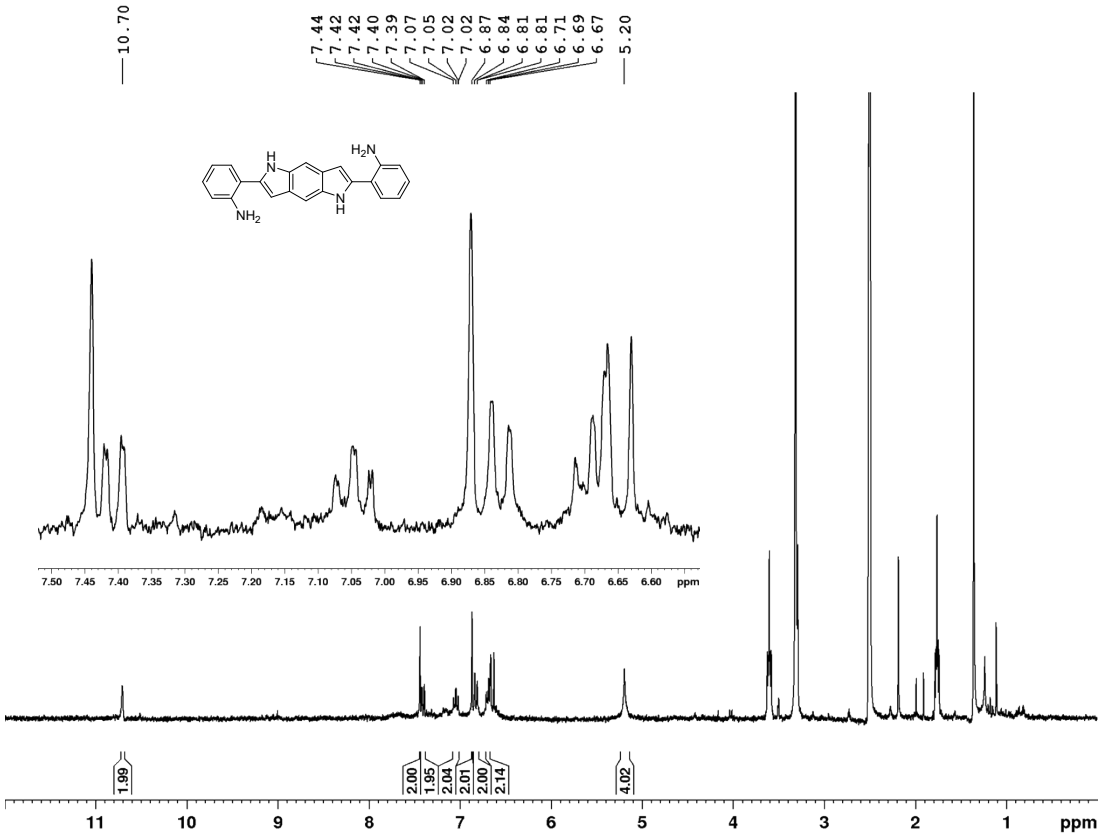


Figure S23. ^{1}H NMR spectrum (301 MHz, DMSO-d_6) of **6**.

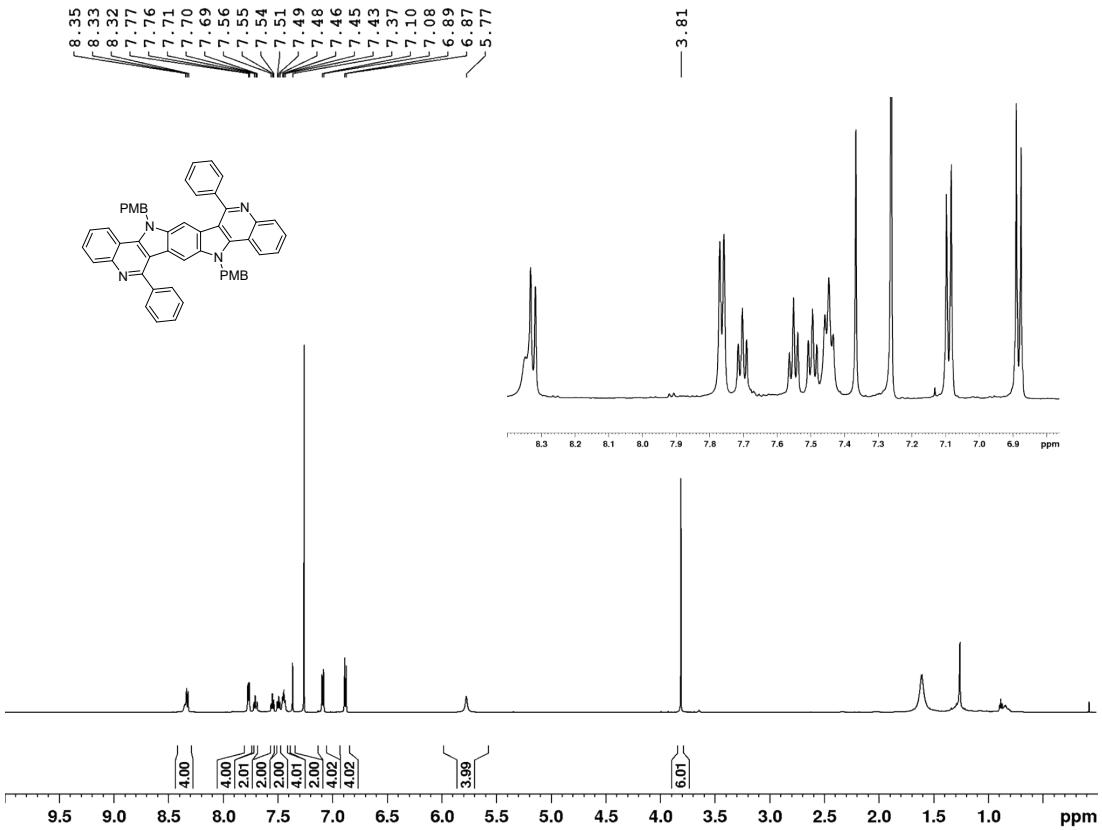


Figure S24. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **7a**.

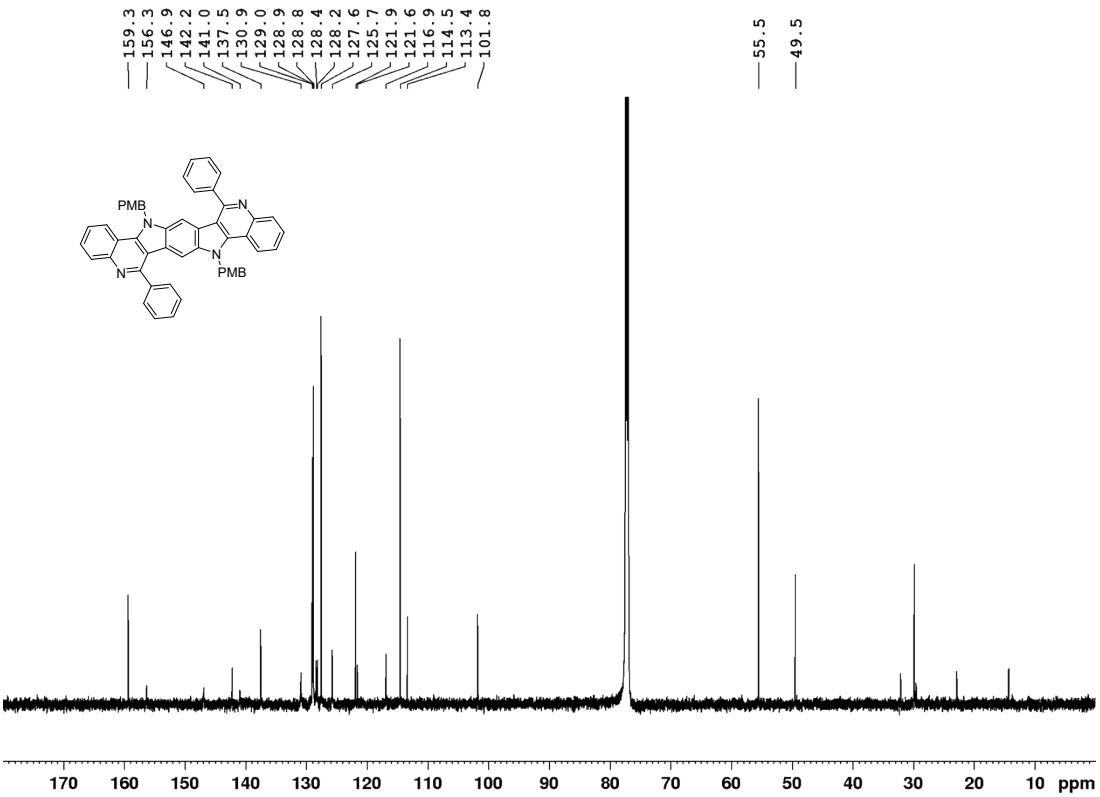


Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **7a**.

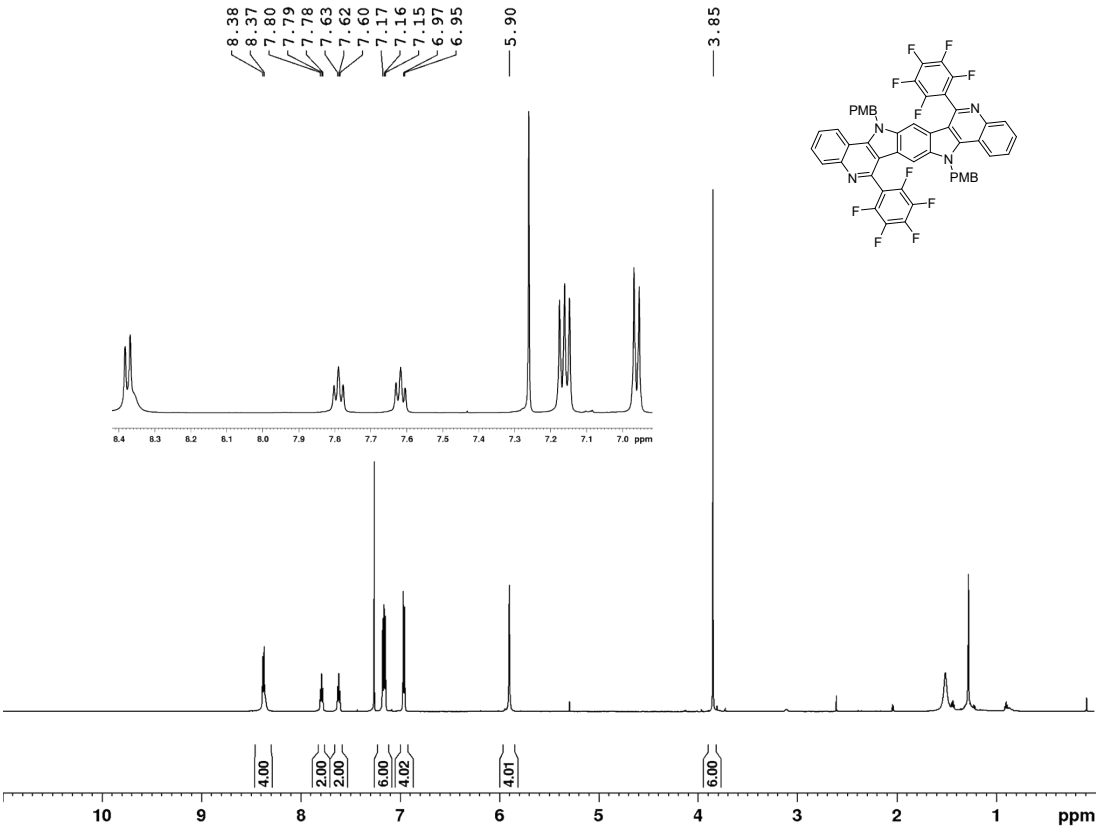


Figure S26. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 50 °C) of **7b**.

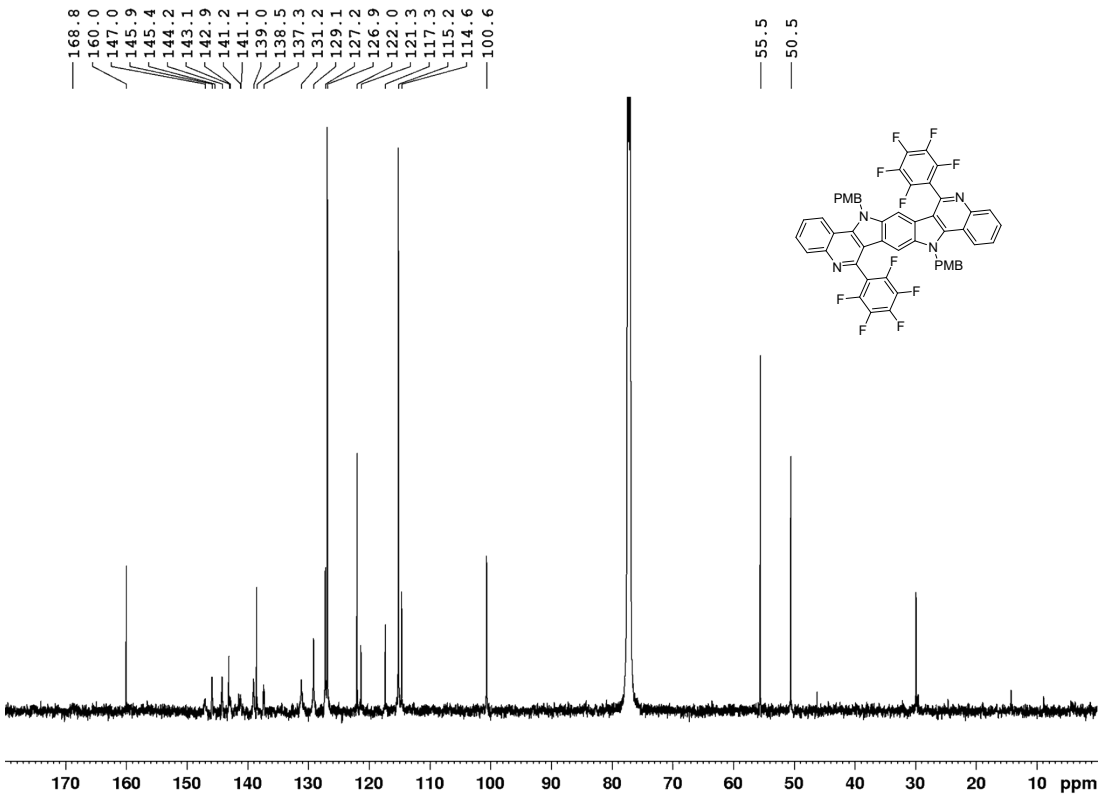


Figure S27. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$, 50 °C) of **7b**.

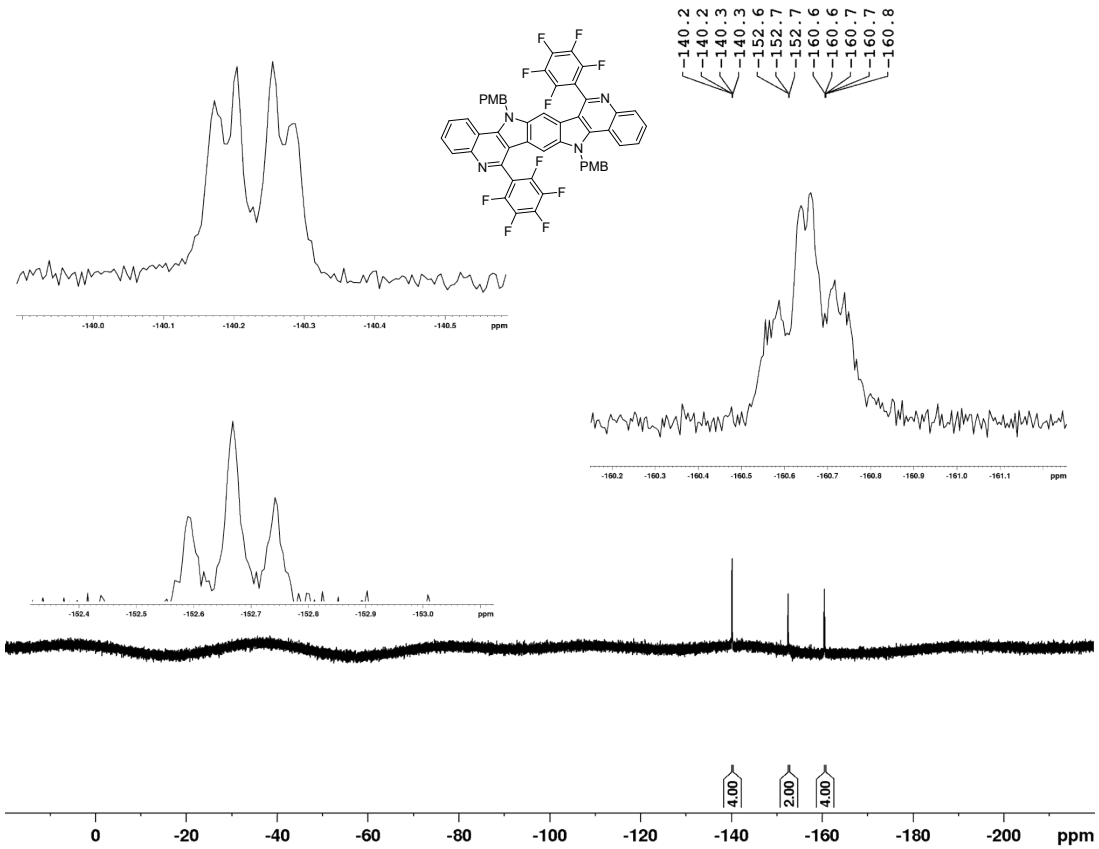


Figure S28. $^{19}F\{^{1}H\}$ NMR spectrum (283 MHz, $CDCl_3$) of **7b**.

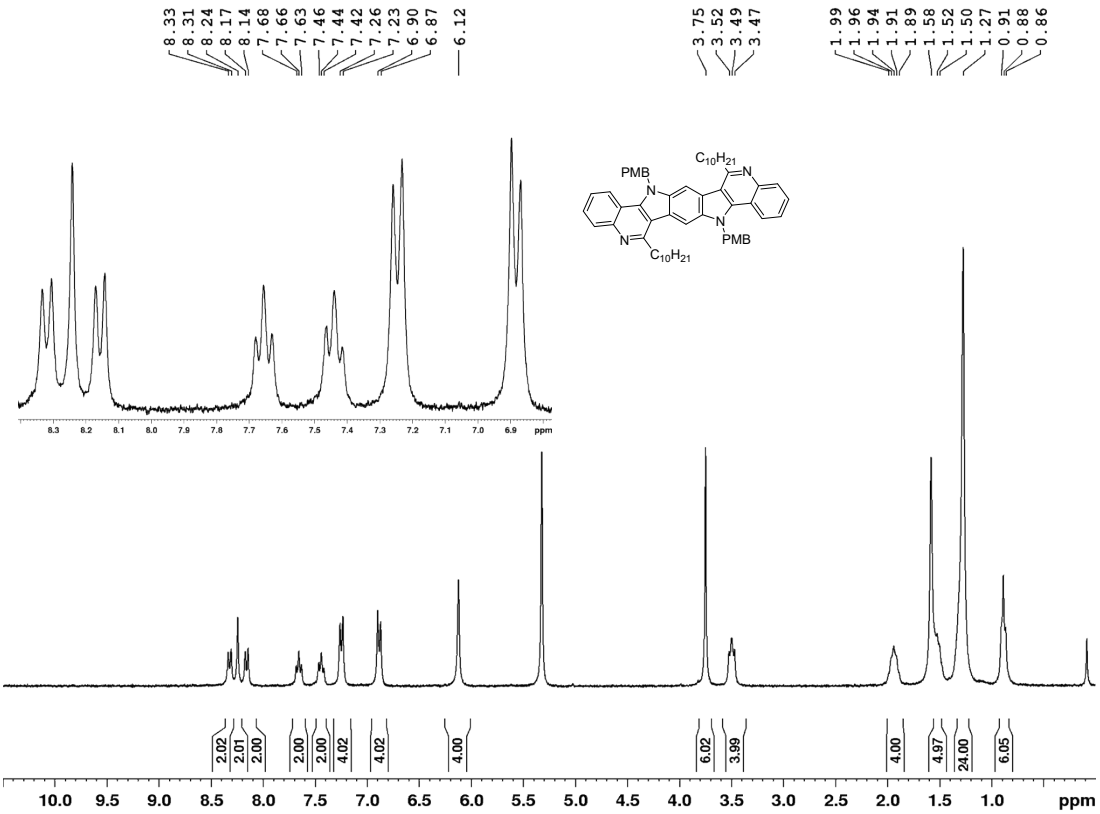


Figure S29. ^{1}H NMR spectrum (301 MHz, CD_2Cl_2) of **7c**.

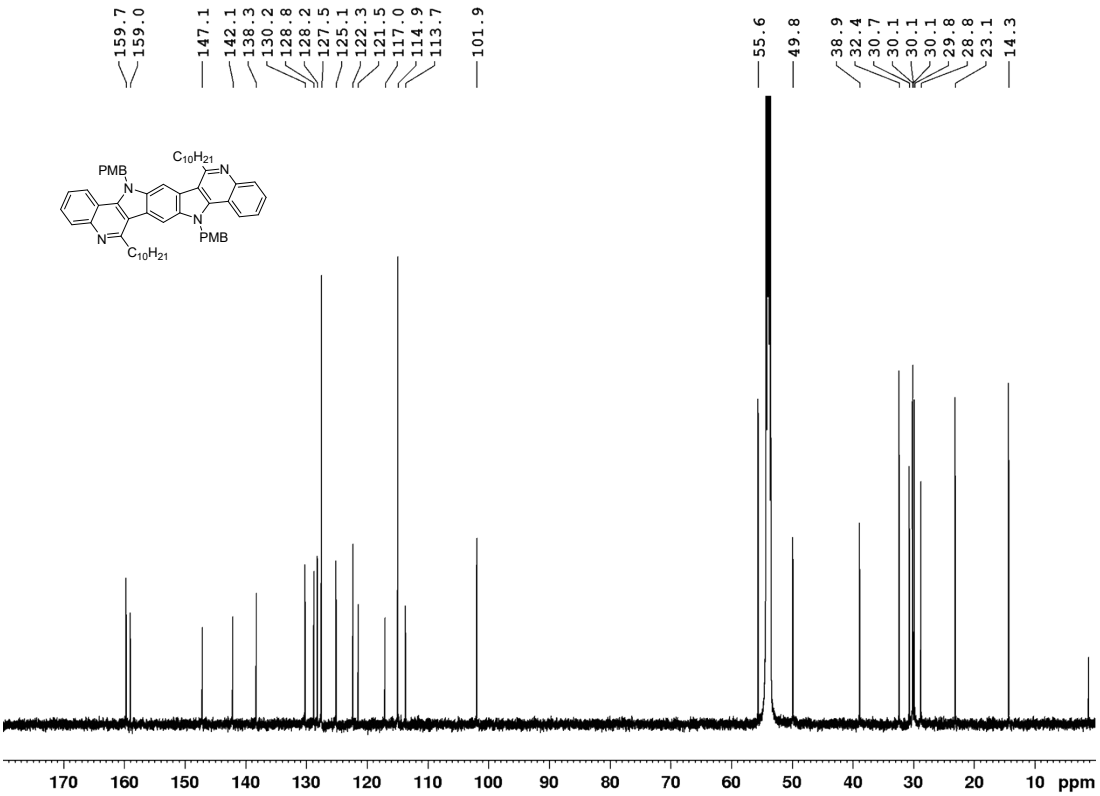


Figure S30. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, CD_2Cl_2) of **7c**.

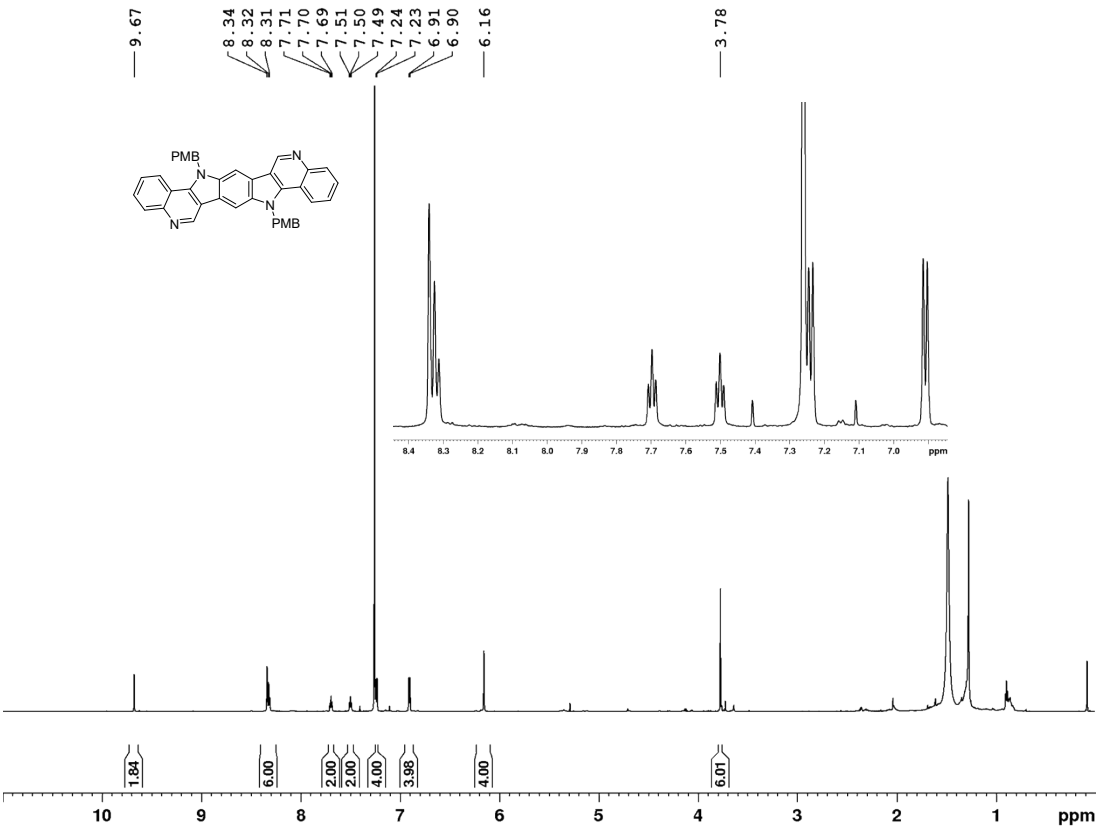


Figure S31. ^{1}H NMR spectrum (700 MHz, $CDCl_3$, 50 °C) of **7d**.

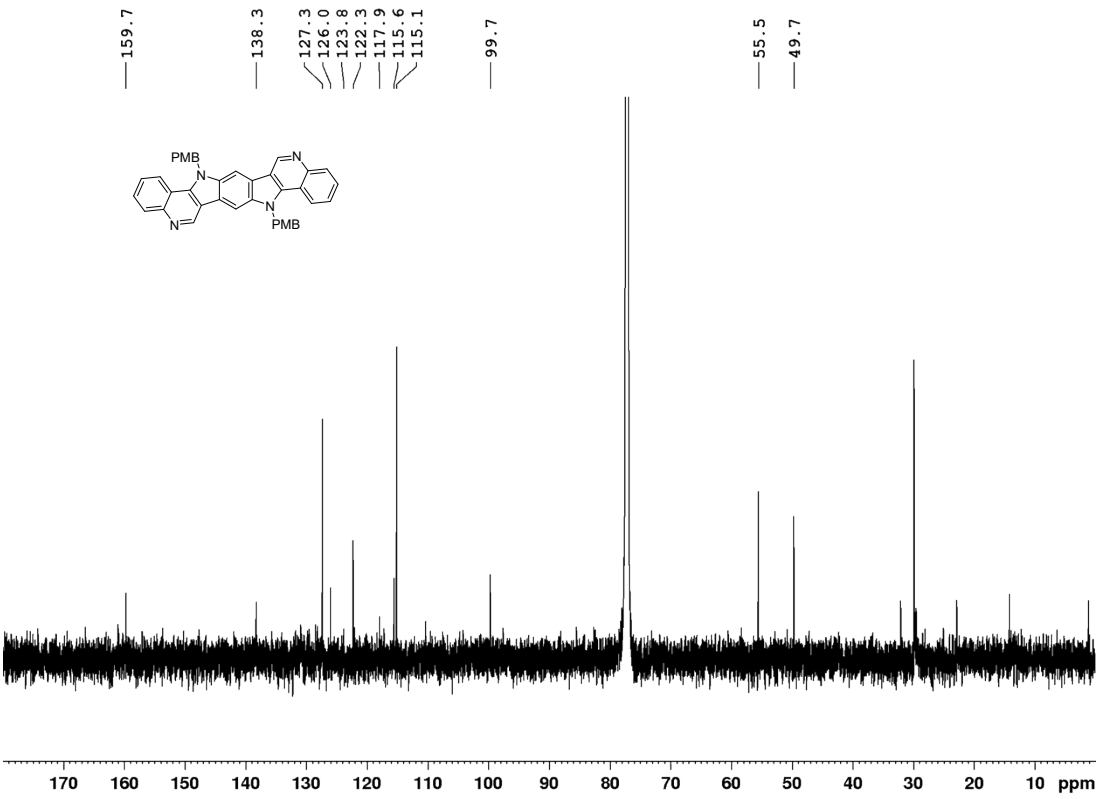


Figure S32. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, $CDCl_3$, 50 °C) of **7d**.

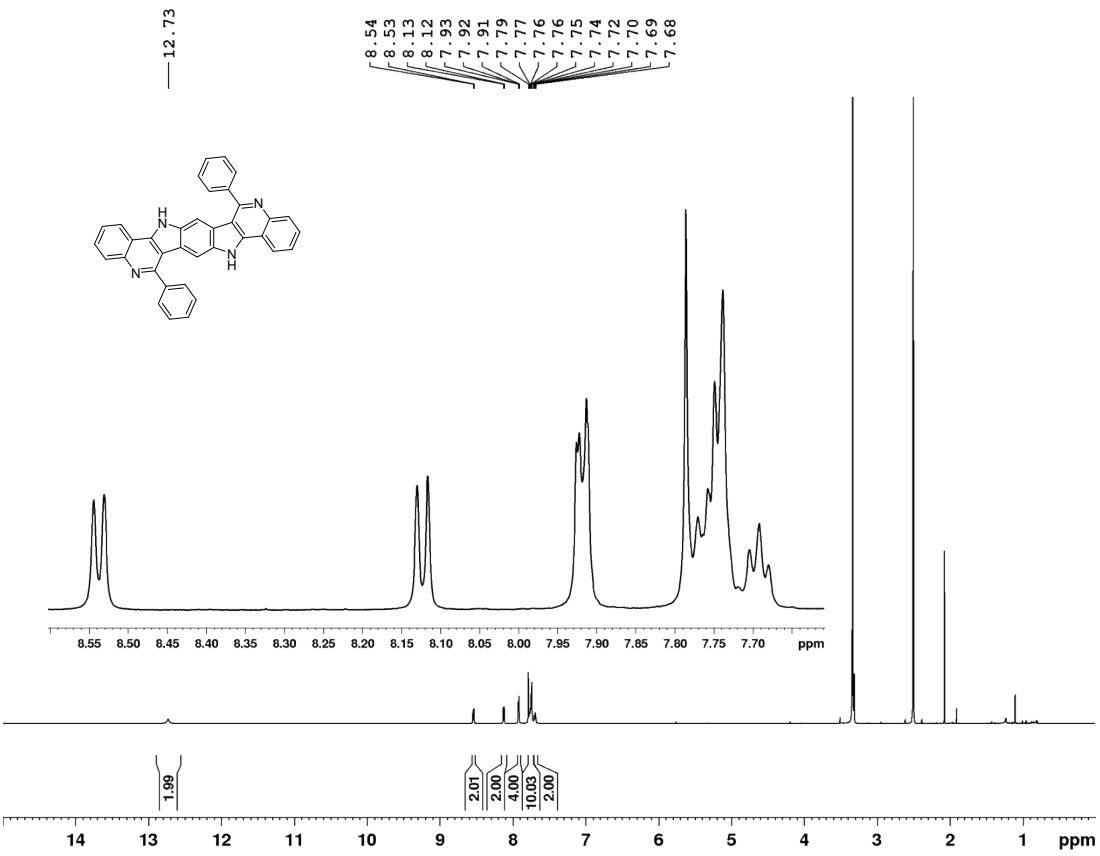


Figure S33. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of **8a**.

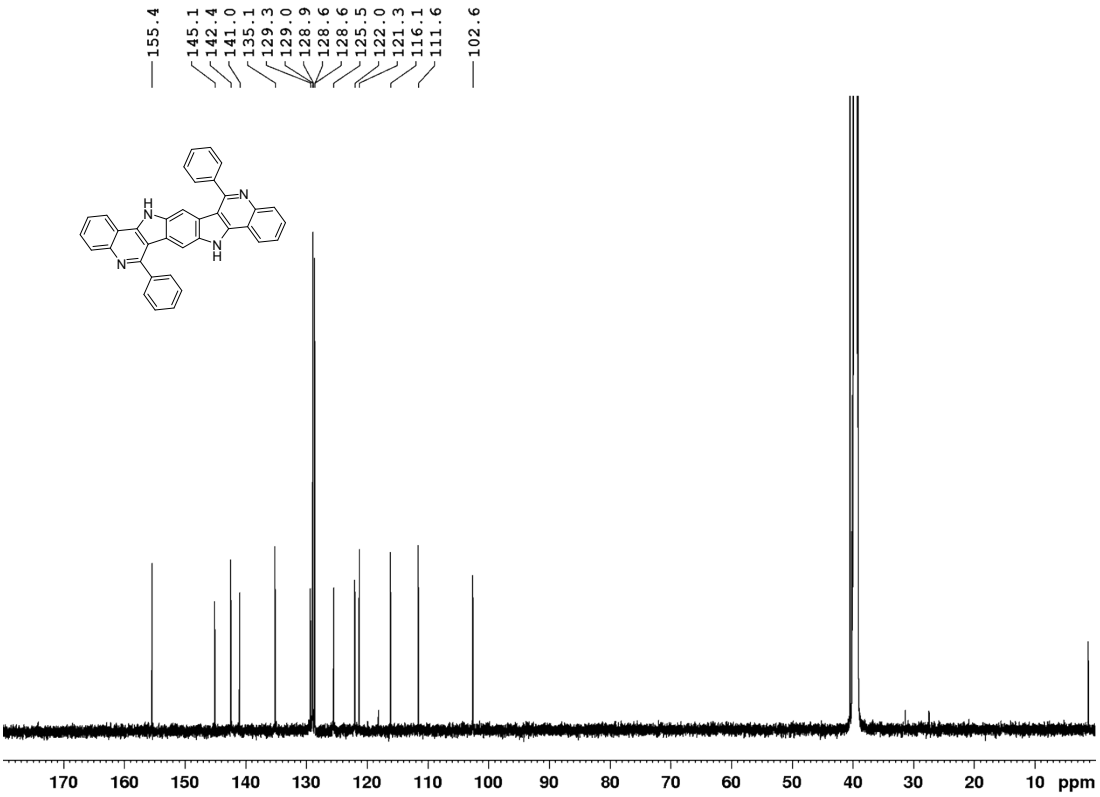


Figure S34. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, DMSO-d_6) of **8a**.

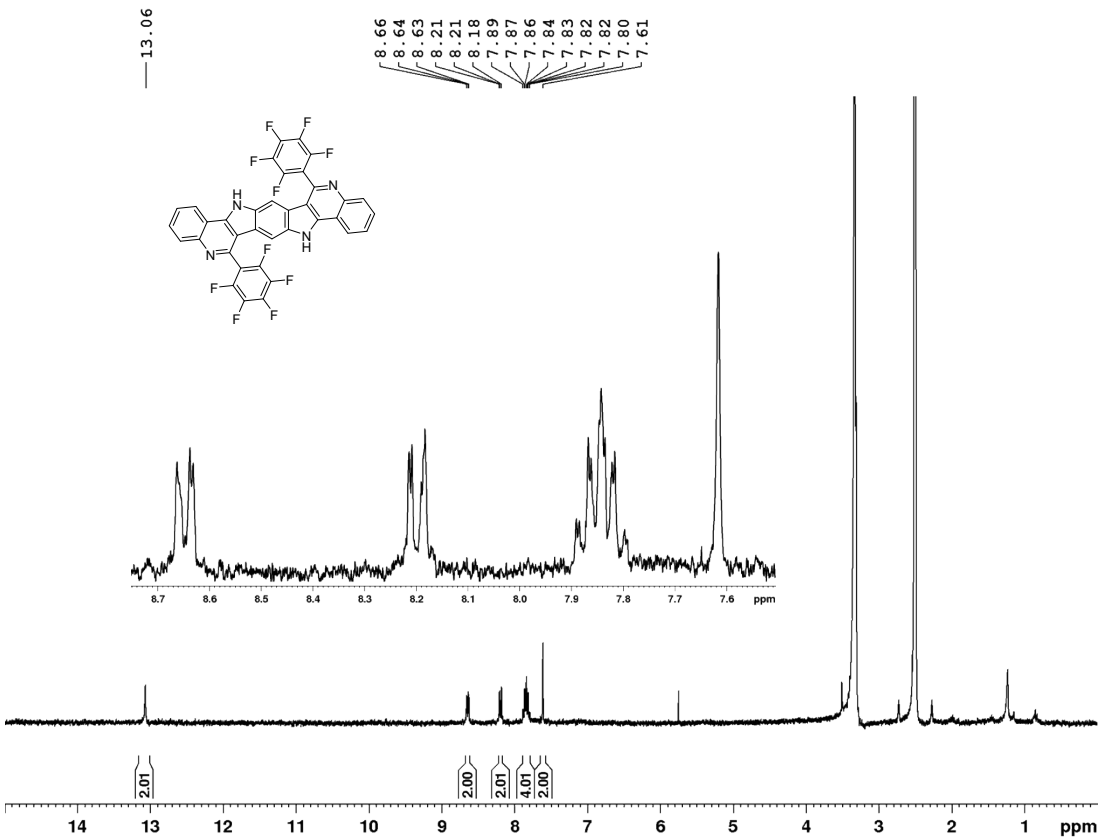


Figure S35. ^{1}H NMR spectrum (301 MHz, DMSO-d_6) of **8b**.

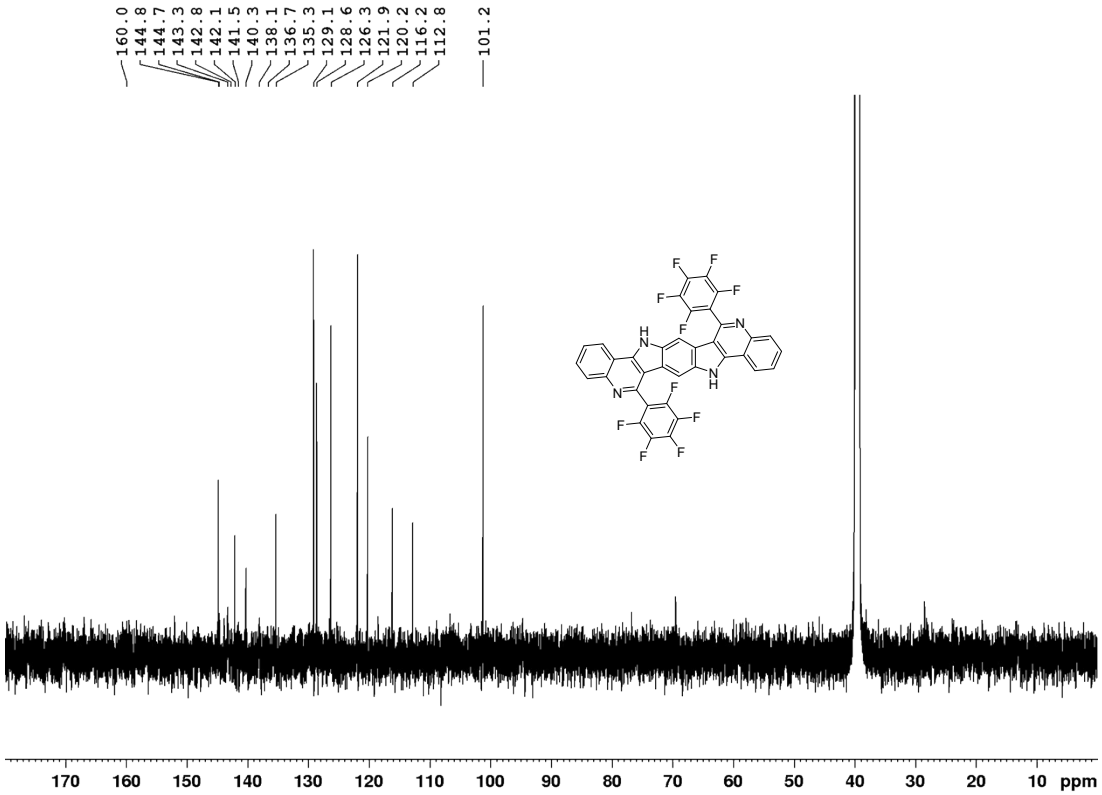


Figure S36. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, DMSO-d_6, 80 °C) of **8b**.

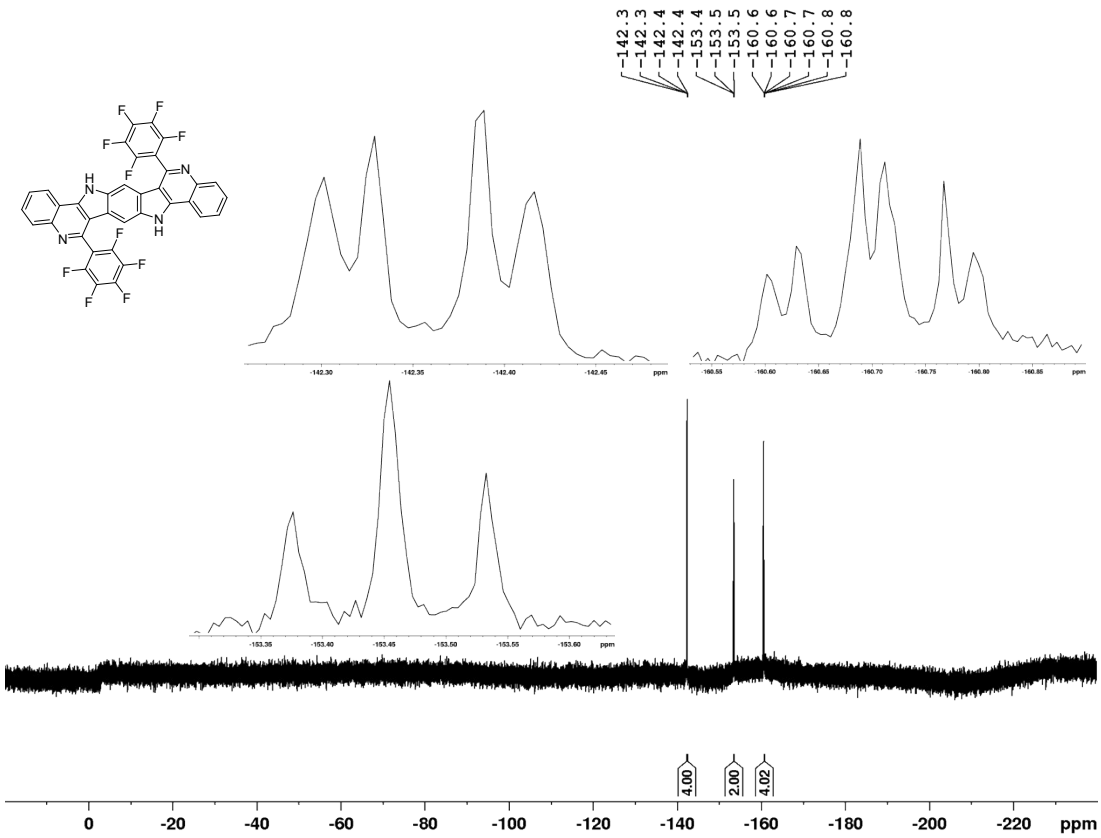


Figure S37. $^{19}F\{^{1}H\}$ NMR spectrum (283 MHz, DMSO-d_6) of **8b**.

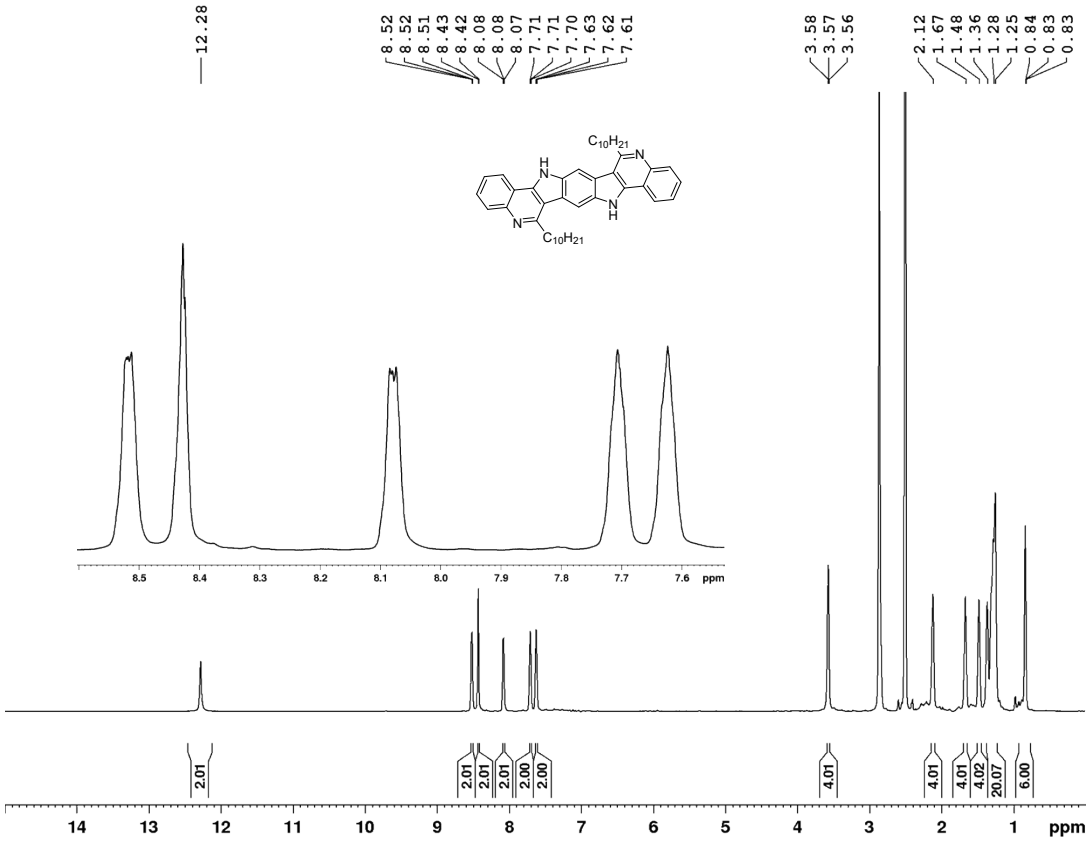


Figure S38. ^{1}H NMR spectrum (700 MHz, DMSO-d_6, 120 °C) of **8c**.

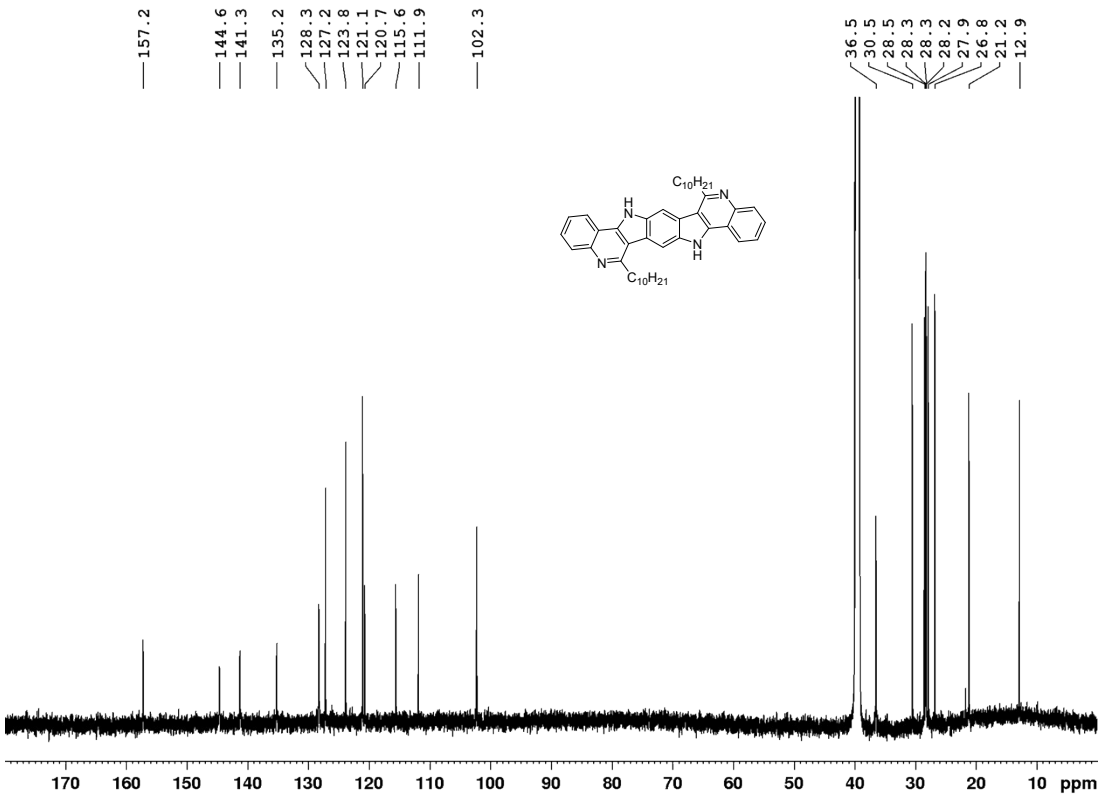


Figure S39. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, DMSO-d_6, 120 °C) of **8c**.

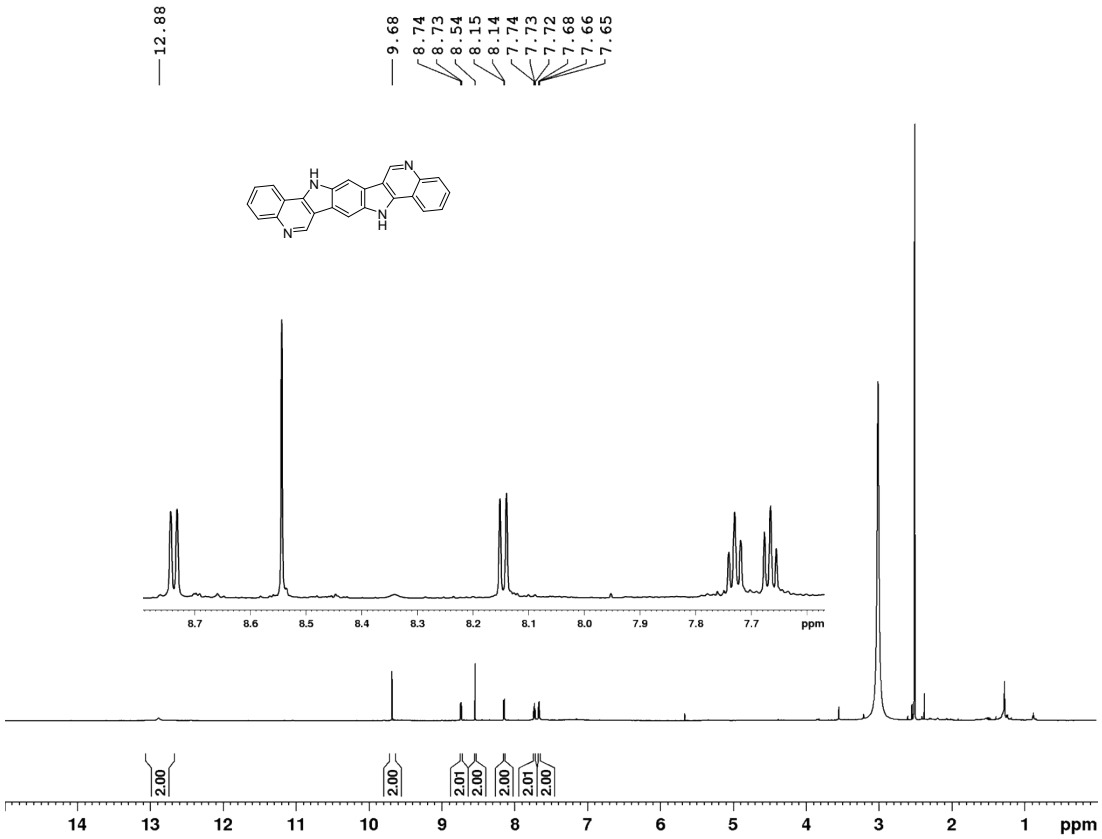


Figure S40. ^{1}H NMR spectrum (700 MHz, DMSO-d_6, 100 °C) of **8d**.

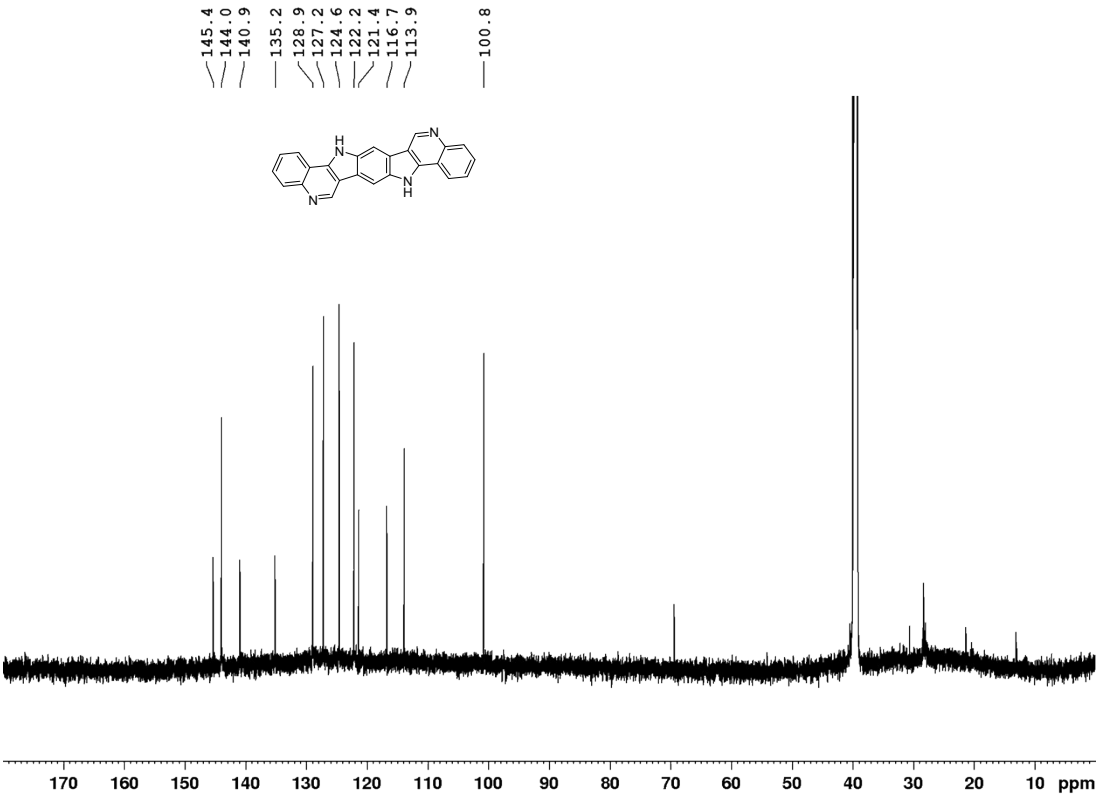


Figure S41. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, DMSO-d_6, 100 °C) of **8d**.

3 **UV-Vis** and Fluorescence Spectra

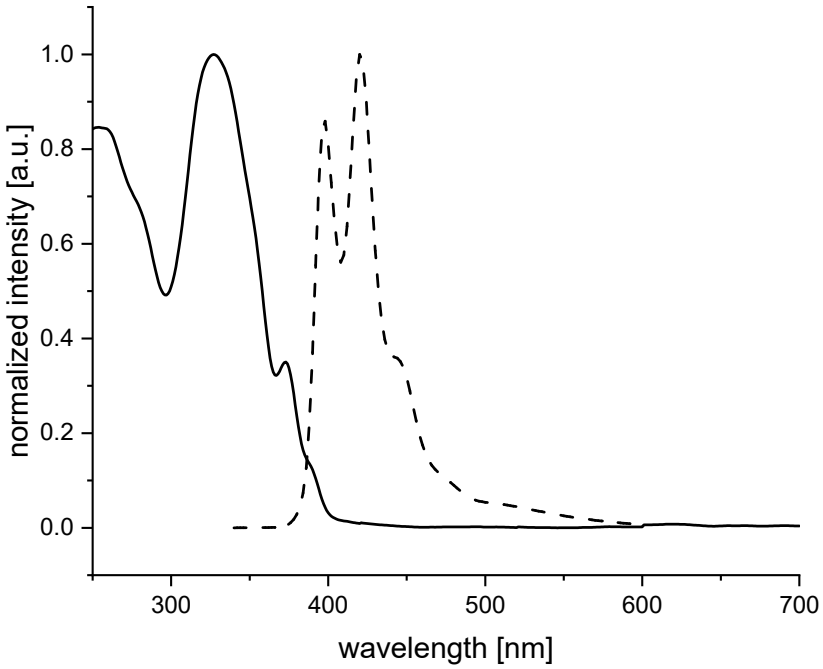


Figure S42. Absorption (solid line) and emission (dashed line) spectra of **2a** in DCM.

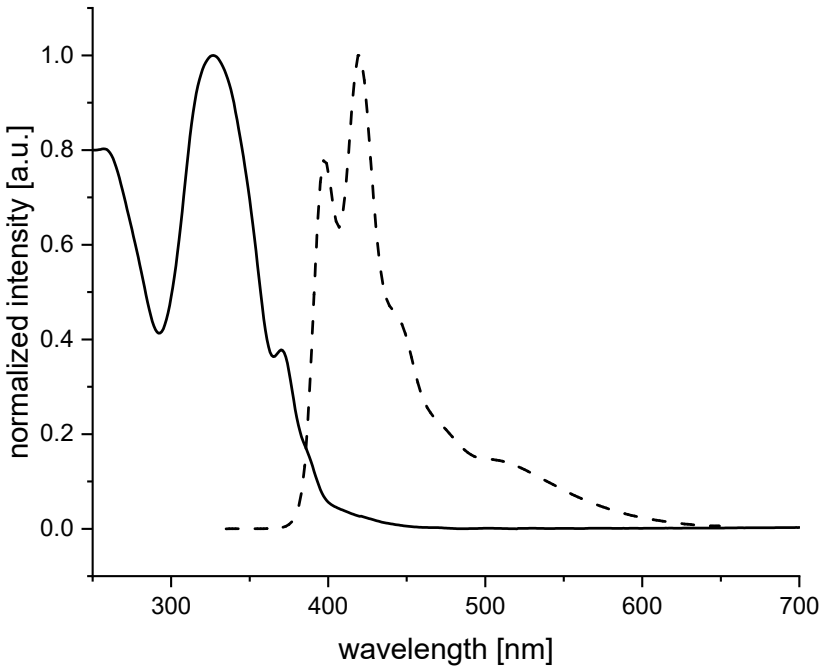


Figure S43. Absorption (solid line) and emission (dashed line) spectra of **2b** in DCM.

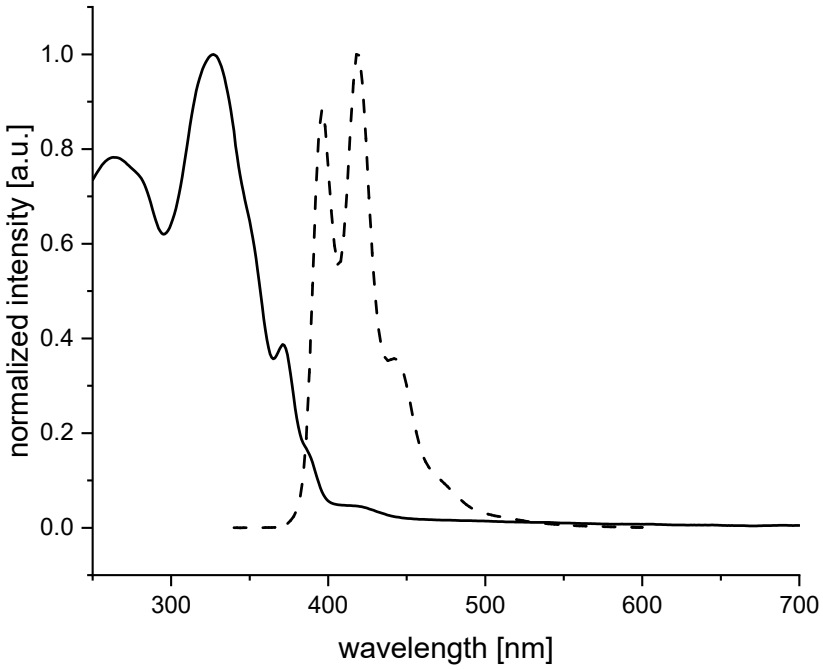


Figure S44. Absorption (solid line) and emission (dashed line) spectra of **2c** in DCM.

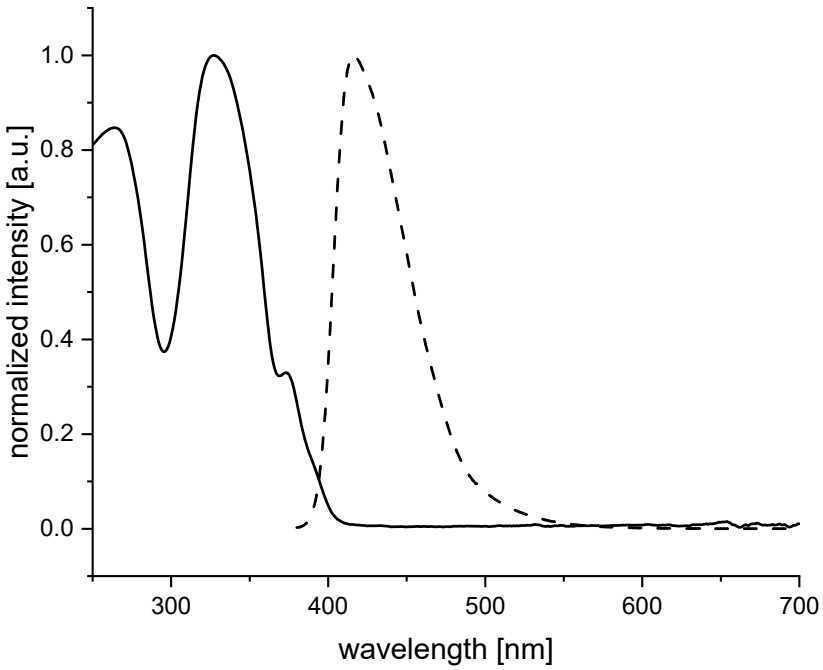


Figure S45. Absorption (solid line) and emission (dashed line) spectra of **2d** in DCM.

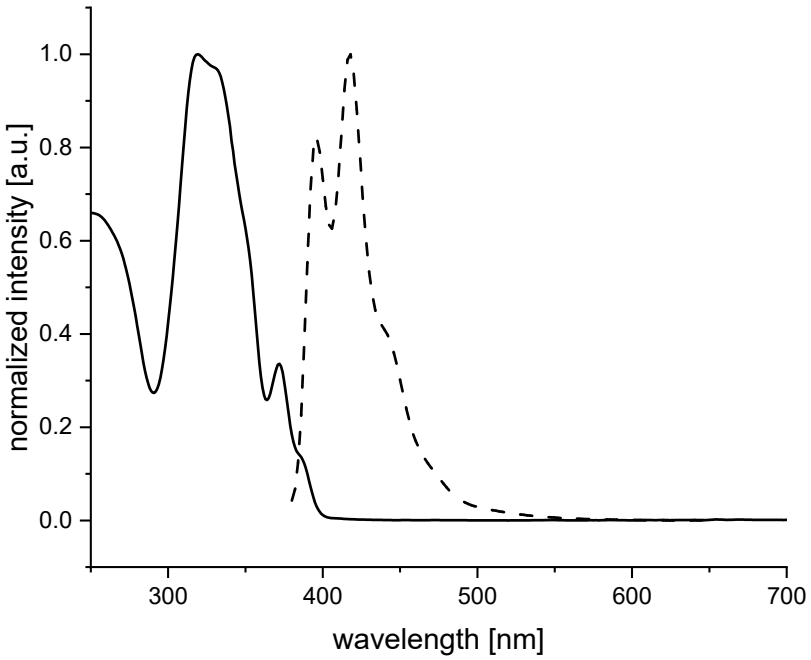


Figure S46. Absorption (solid line) and emission (dashed line) spectra of **2e** in DCM.

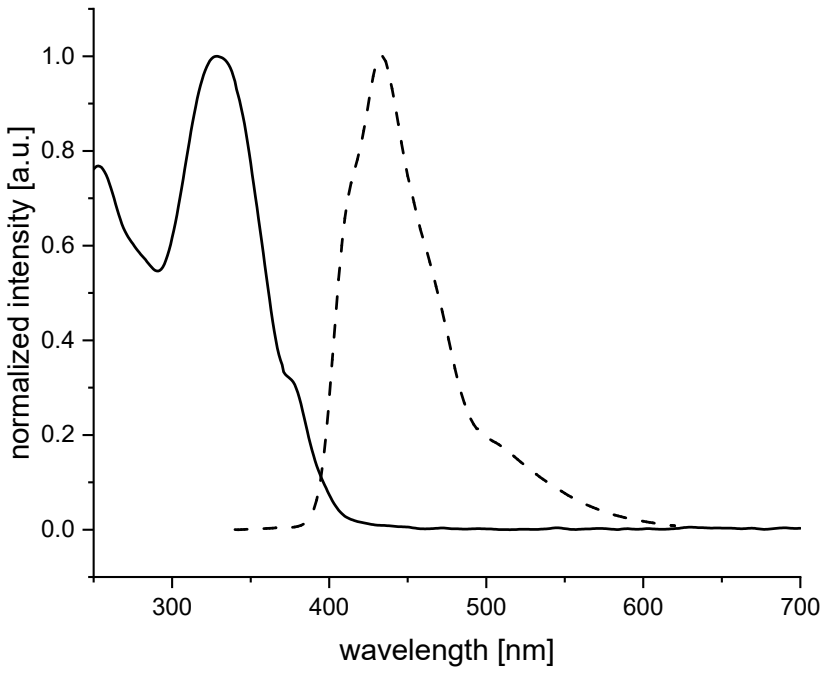


Figure S47. Absorption (solid line) and emission (dashed line) spectra of **2f** in DCM.

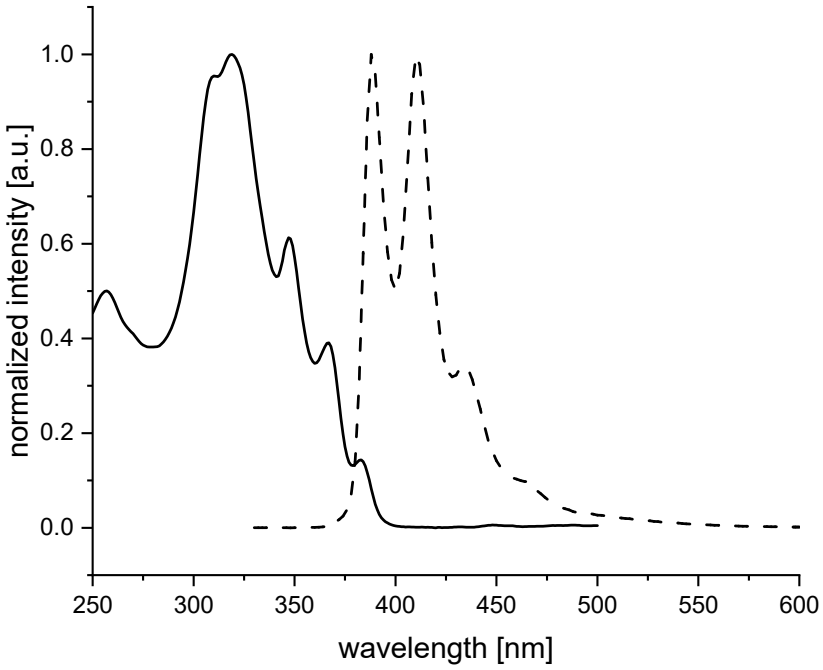


Figure S48. Absorption (solid line) and emission (dashed line) spectra of **2g** in DCM.

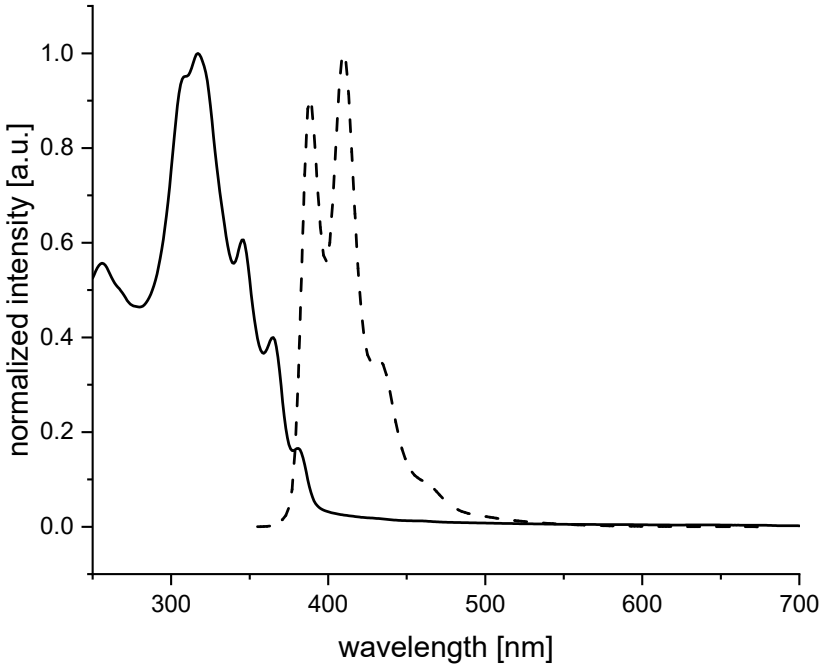


Figure S49. Absorption (solid line) and emission (dashed line) spectra of **2h** in DCM.

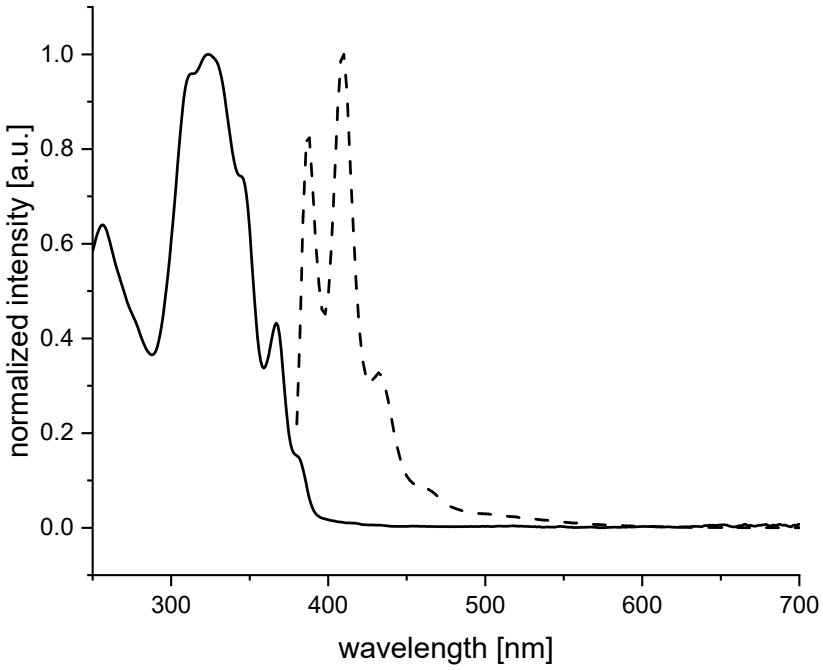


Figure S50. Absorption (solid line) and emission (dashed line) spectra of **2i** in DCM.

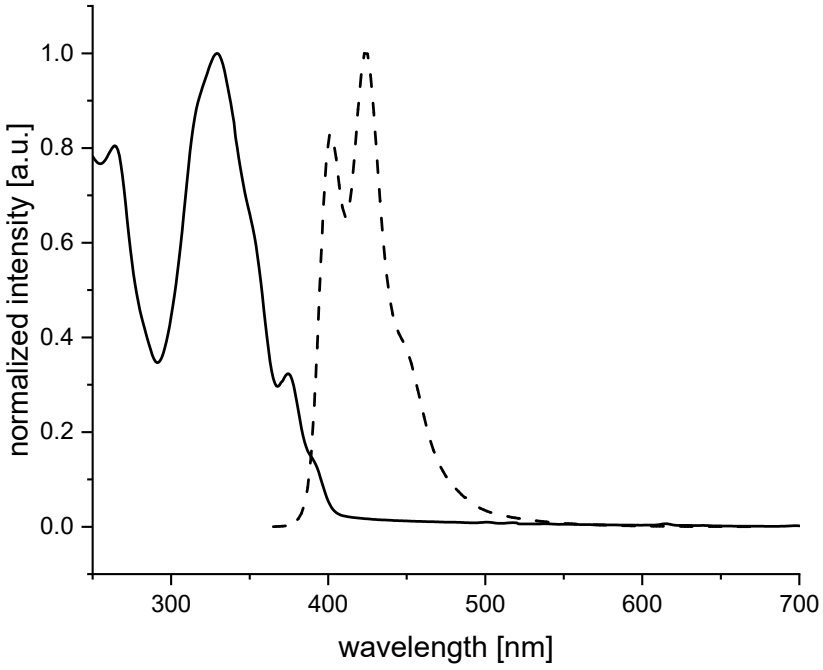


Figure S51. Absorption (solid line) and emission (dashed line) spectra of **7a** in DCM.

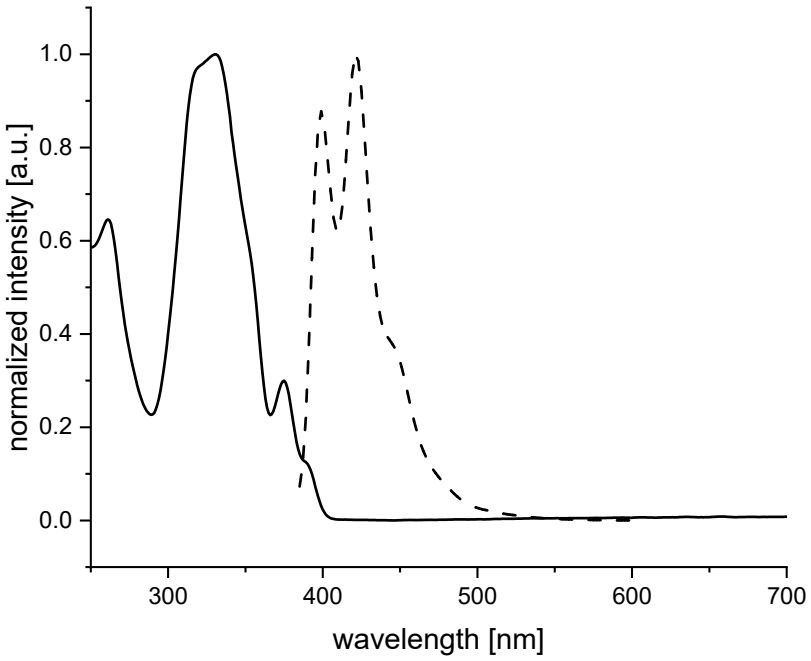


Figure S52. Absorption (solid line) and emission (dashed line) spectra of **7b** in DCM.

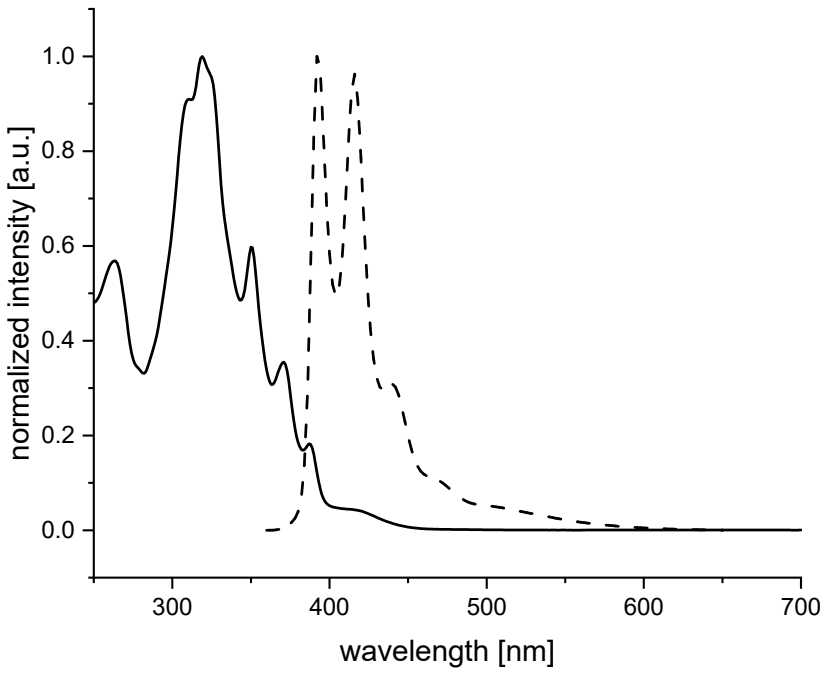


Figure S53. Absorption (solid line) and emission (dashed line) spectra of **7c** in DCM.

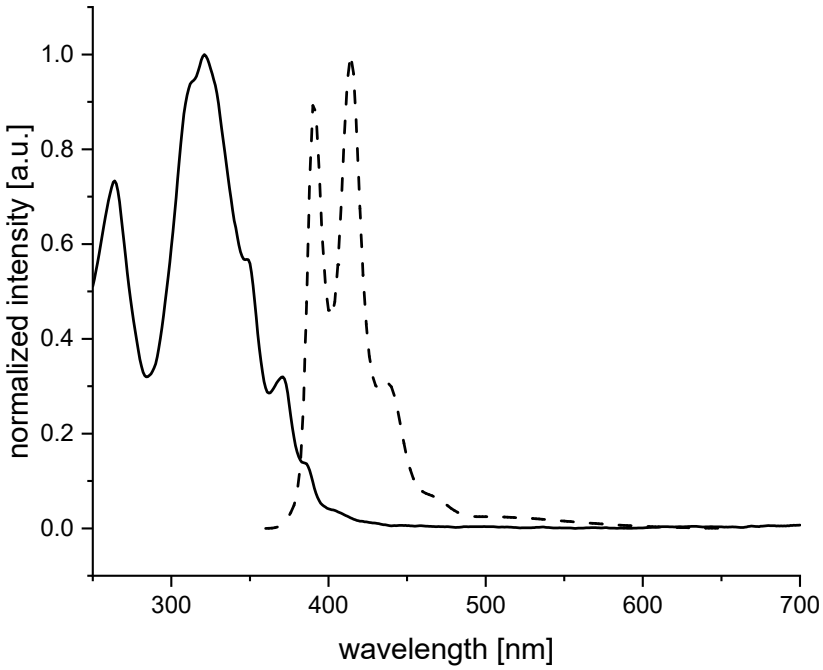


Figure S54. Absorption (solid line) and emission (dashed line) spectra of **7d** in DCM.

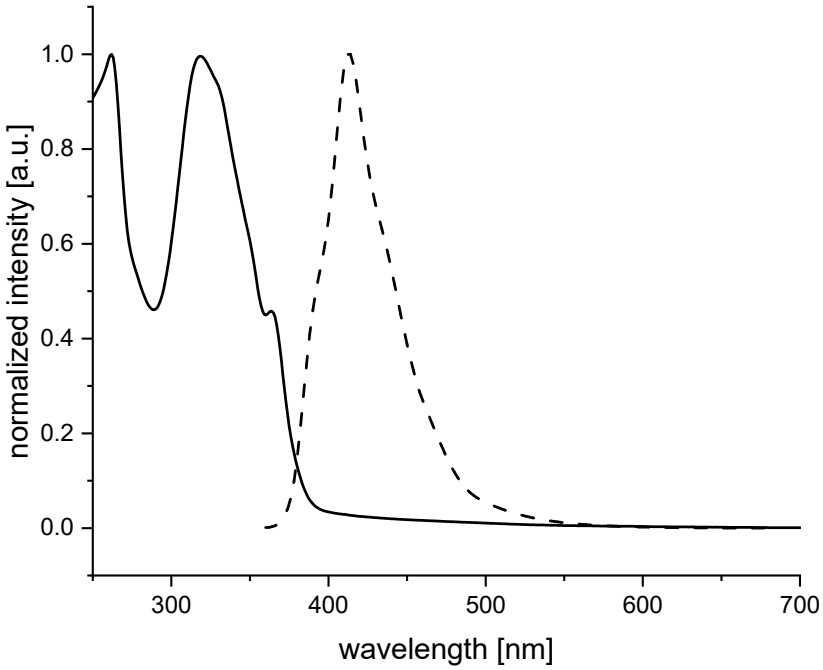


Figure S55. Absorption (solid line) and emission (dashed line) spectra of **8a** in DCM.

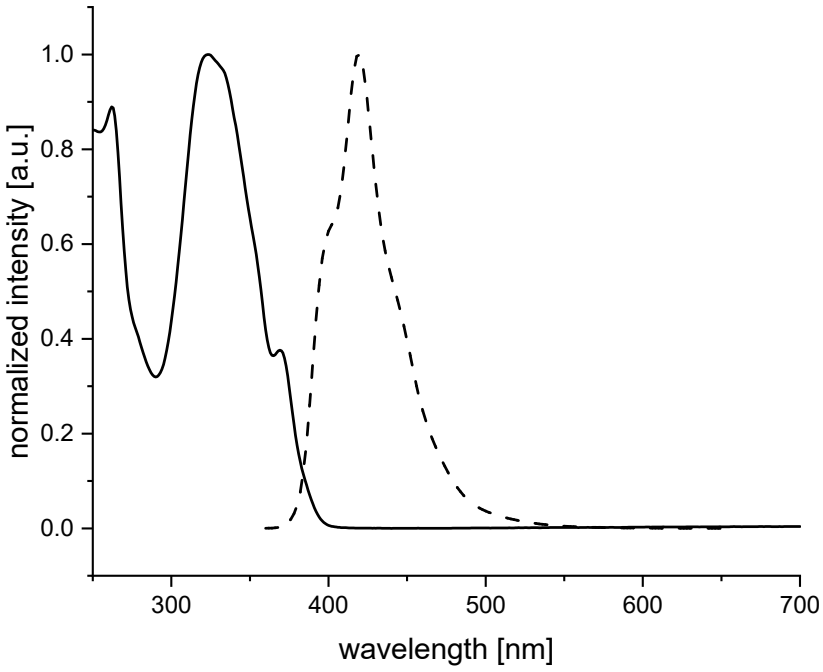


Figure S56. Absorption (solid line) and emission (dashed line) spectra of **8a** in THF.

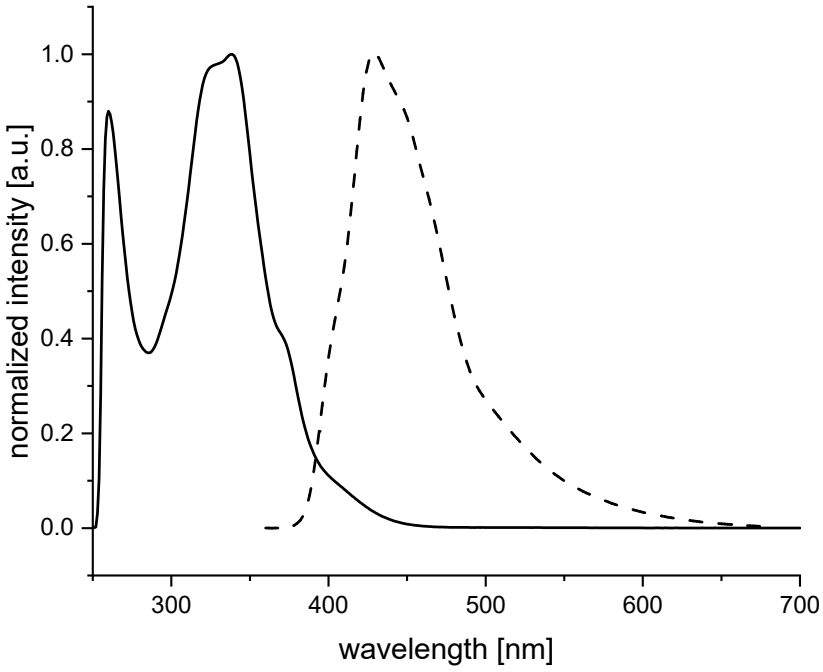


Figure S57. Absorption (solid line) and emission (dashed line) spectra of **8a** in DMSO.

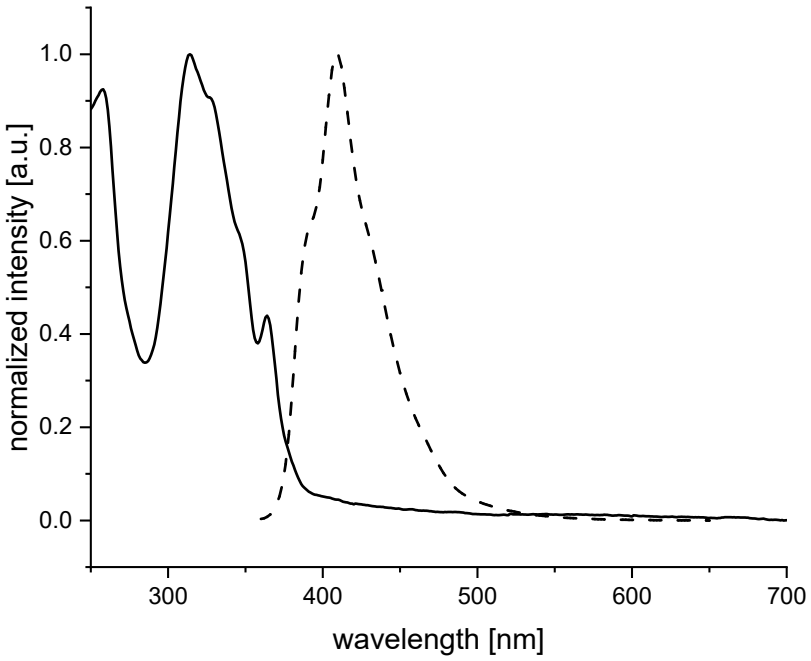


Figure S58. Absorption (solid line) and emission (dashed line) spectra of **8b** in DCM.

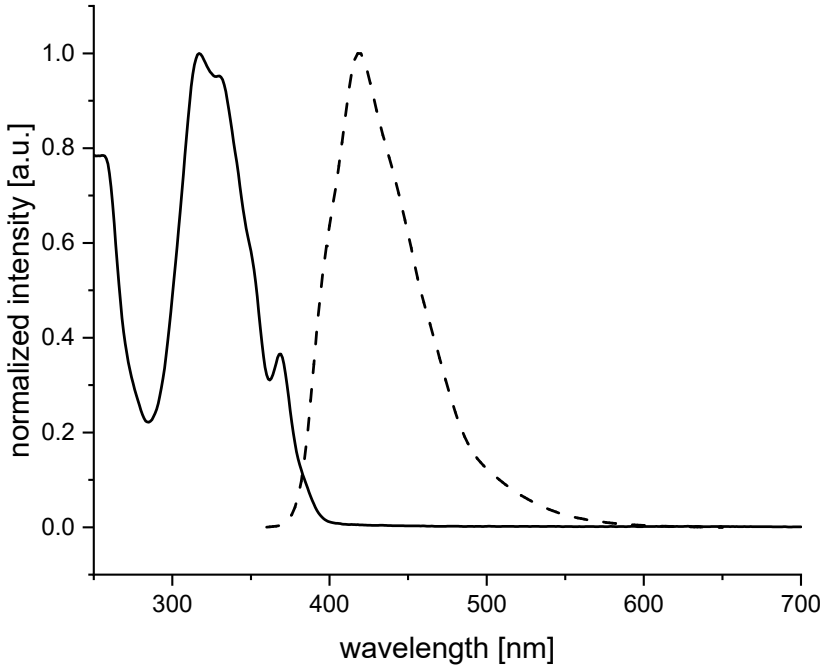


Figure S59. Absorption (solid line) and emission (dashed line) spectra of **8b** in THF.

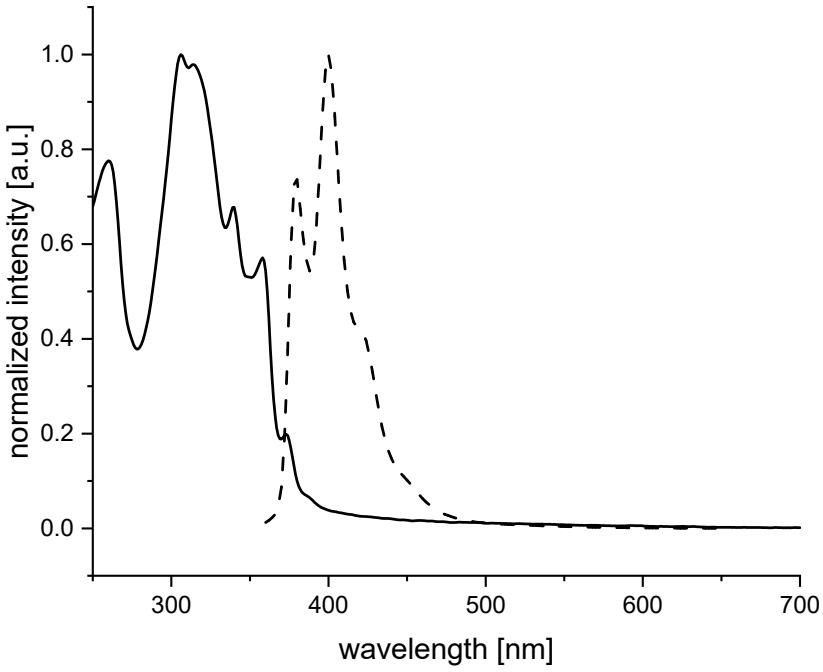


Figure S60. Absorption (solid line) and emission (dashed line) spectra of **8c** in DCM.

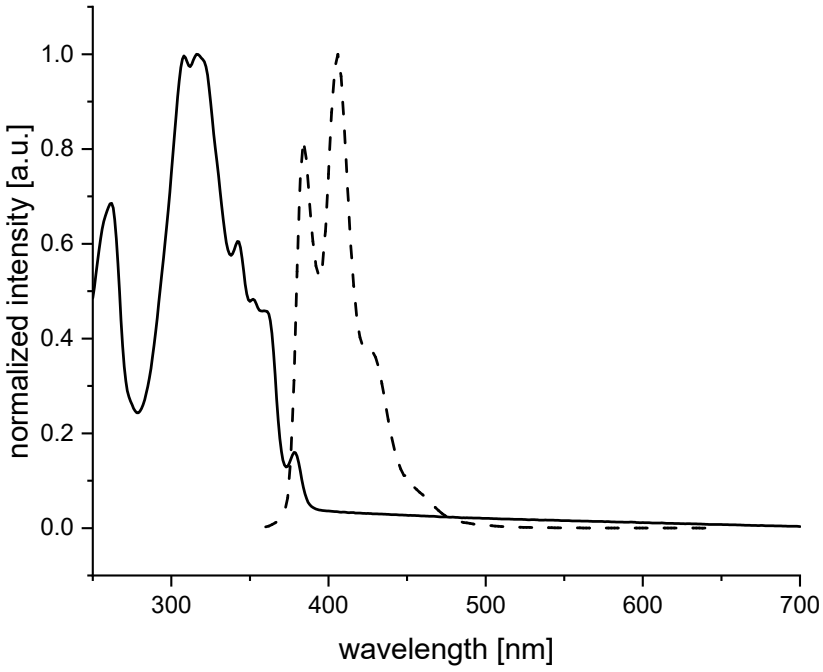


Figure S61. Absorption (solid line) and emission (dashed line) spectra of **8c** in THF.

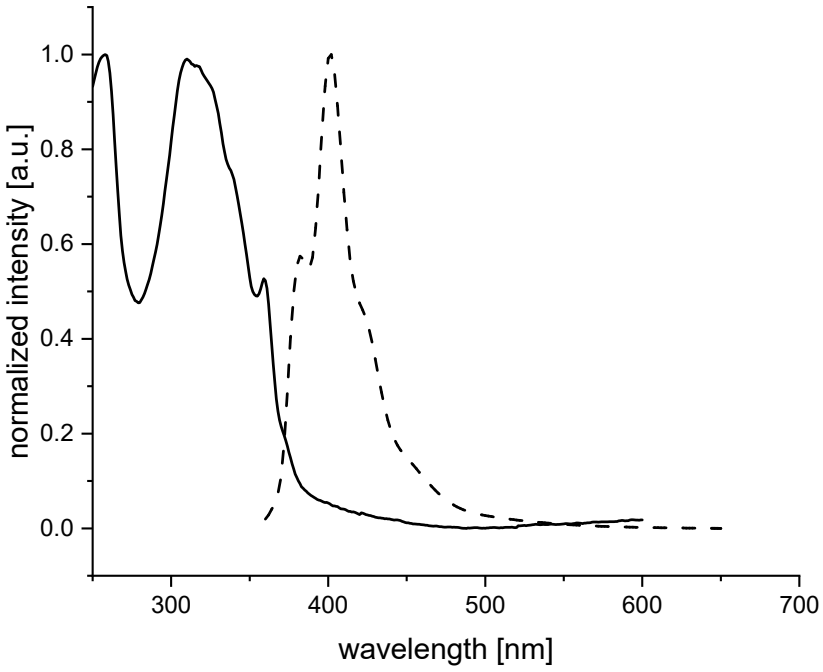


Figure S62. Absorption (solid line) and emission (dashed line) spectra of **8d** in DCM.

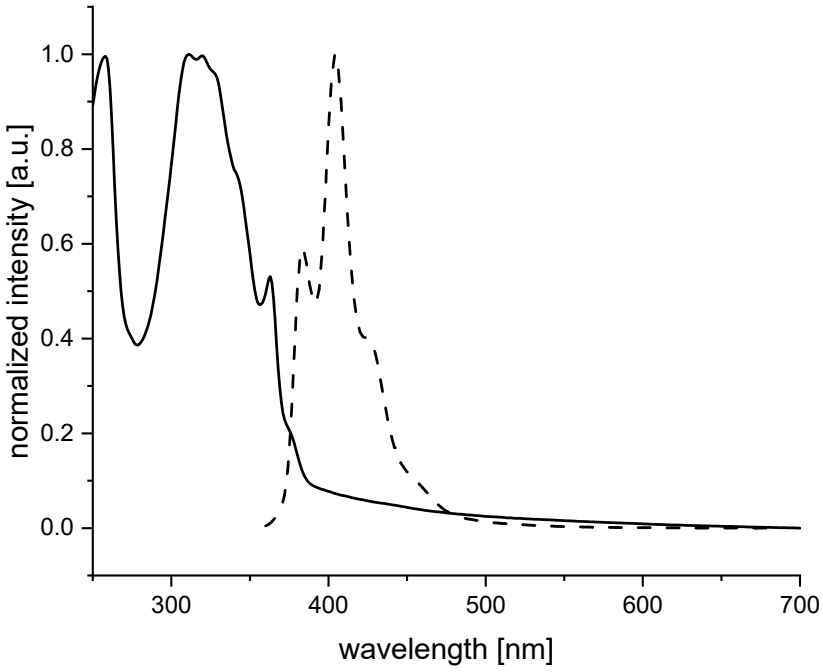


Figure S63. Absorption (solid line) and emission (dashed line) spectra of **8d** in THF.

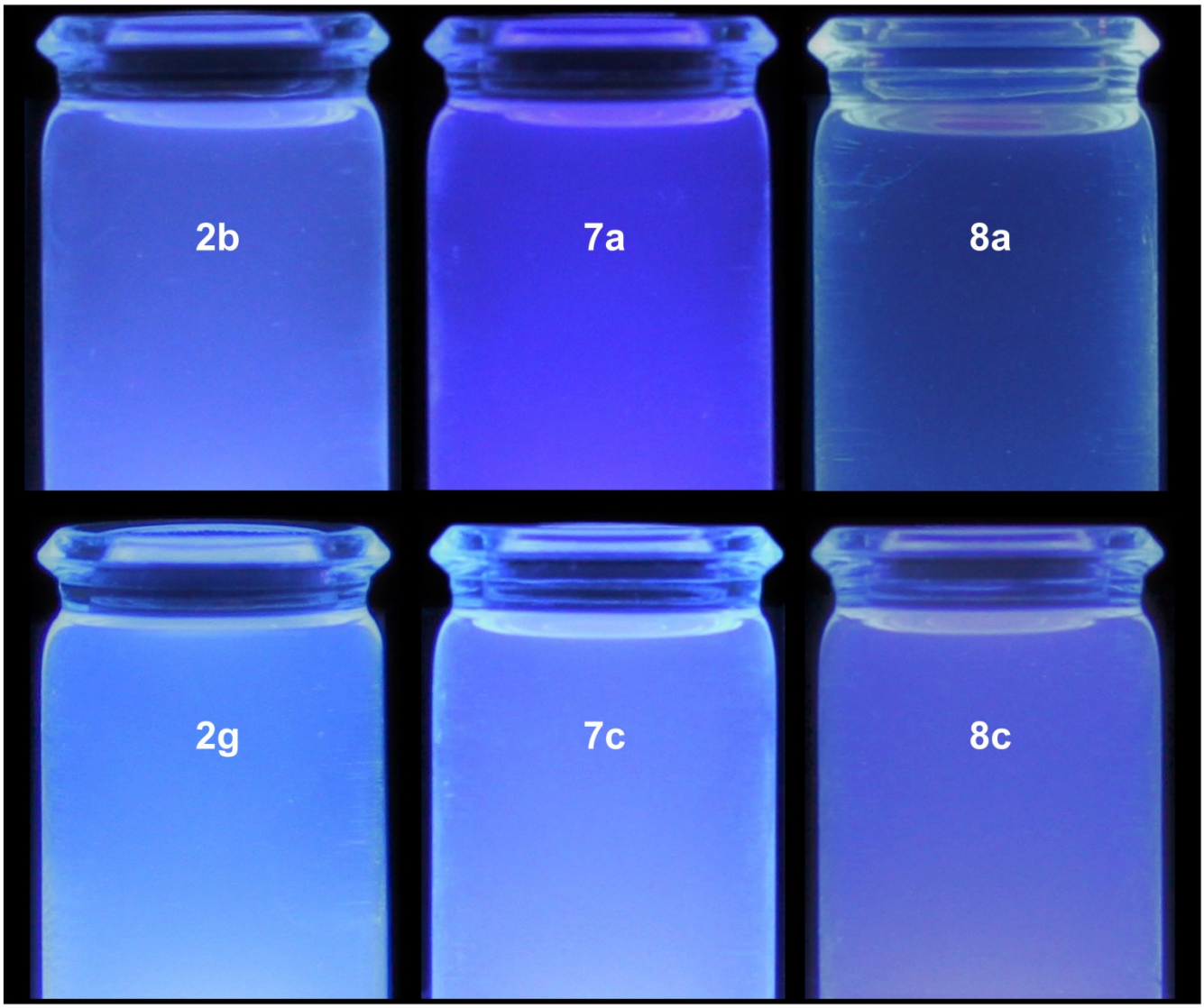
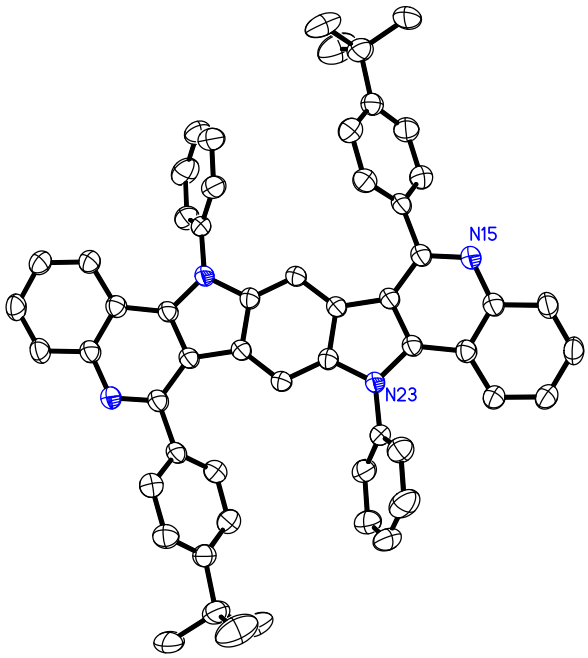


Figure S64. Photographs of selected compounds as solution in DCM under irradiation by UV light (365 nm).

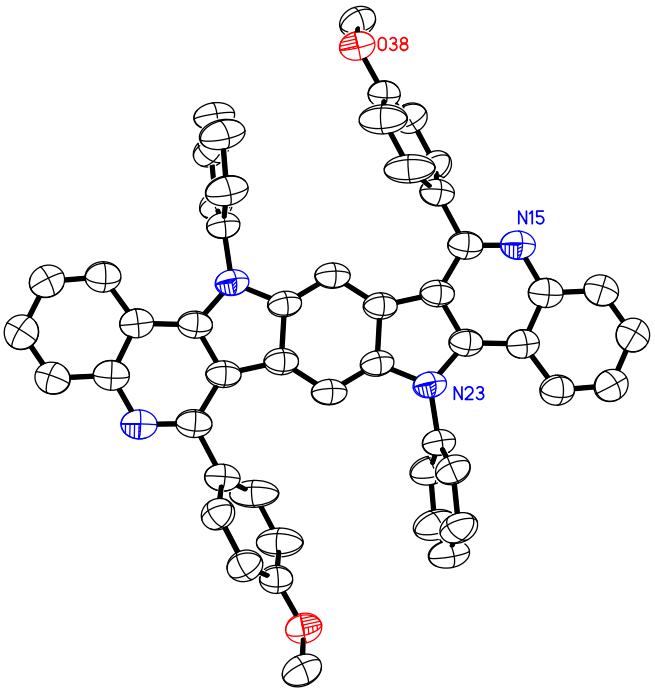
4 Crystallographic Data

Table S2. Crystal structure, crystal data and structure refinement of **2a** (2205008).



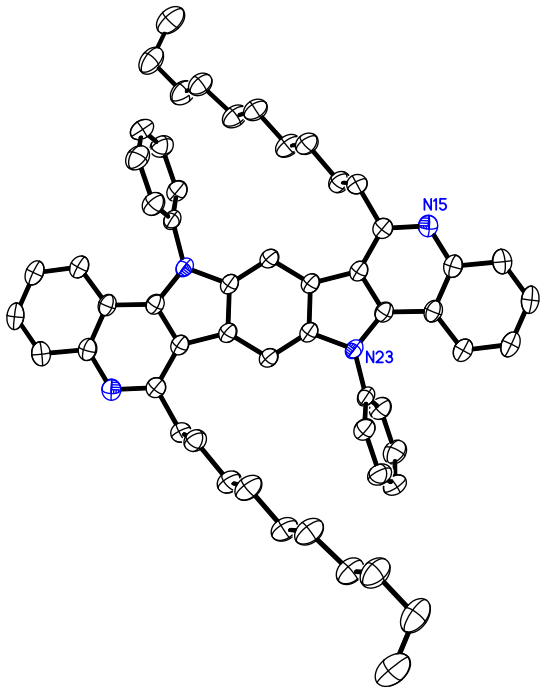
Empirical formula	$C_{56}H_{46}N_4$	
Formula weight	774.97	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Z	2	
Unit cell dimensions	a = 9.3971(4) Å	α = 90 deg.
	b = 11.2369(4) Å	β = 91.402(4) deg.
	c = 19.4152(10) Å	γ = 90 deg.
Volume	2049.52(16) $Å^3$	
Density (calculated)	1.26 g/cm^3	
Absorption coefficient	0.56 mm^{-1}	
Crystal shape	needle	
Crystal size	0.190 x 0.030 x 0.027 mm^3	
Crystal colour	yellow	
Theta range for data collection	4.5 to 67.1 deg.	
Index ranges	$-11 \le h \le 5$, $-11 \le k \le 13$, $-22 \le l \le 22$	
Reflections collected	12146	
Independent reflections	3572 (R(int) = 0.0608)	
Observed reflections	2135 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.29 and 0.74	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	3572 / 314 / 302	
Goodness-of-fit on F^2	1.03	
Final R indices (I>2sigma(I))	R1 = 0.055, wR2 = 0.114	
Largest diff. peak and hole	0.25 and -0.19 $eÅ^{-3}$	

Table S3. Crystal structure, crystal data and structure refinement of **2c** (2205009).



Empirical formula	$C_{50}H_{34}N_4O_2$
Formula weight	722.81
Temperature	200(2) K
Wavelength	1.54178 Å
Crystal system	monoclinic
Space group	C2/c
Z	4
Unit cell dimensions	a = 18.2588(10) Å α = 90 deg. b = 7.7639(3) Å β = 108.351(4) deg. c = 27.0581(19) Å γ = 90 deg.
Volume	3640.7(4) $Å^3$
Density (calculated)	1.32 g/cm^3
Absorption coefficient	0.64 mm^{-1}
Crystal shape	plate
Crystal size	0.600 x 0.127 x 0.010 mm^3
Crystal colour	pale Yellow
Theta range for data collection	5.1 to 67.2 deg.
Index ranges	$-21 \le h \le 19$, $-9 \le k \le 5$, $-30 \le l \le 32$
Reflections collected	10345
Independent reflections	3138 (R(int) = 0.0500)
Observed reflections	1891 ($I > 2\sigma(I)$)
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.49 and 0.73
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3138 / 0 / 254
Goodness-of-fit on F^2	1.02
Final R indices (I>2sigma(I))	R1 = 0.054, wR2 = 0.121
Largest diff. peak and hole	0.16 and -0.16 $eÅ^{-3}$

Table S4. Crystal structure, crystal data and structure refinement of **2g** (2205010).



Empirical formula	$C_{56}H_{62}N_4$	
Formula weight	791.09	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Z	2	
Unit cell dimensions	a = 8.2372(2) Å	α = 90 deg.
	b = 17.6098(5) Å	β = 104.397(2) deg.
	c = 15.9665(4) Å	γ = 90 deg.
Volume	2243.30(10) $Å^3$	
Density (calculated)	1.17 g/cm^3	
Absorption coefficient	0.51 mm^{-1}	
Crystal shape	pole	
Crystal size	0.251 x 0.052 x 0.050 mm^3	
Crystal colour	pale yellow	
Theta range for data collection	5.0 to 72.1 deg.	
Index ranges	$-9\leq h\leq 6$, $-18\leq k\leq 21$, $-16\leq l\leq 19$	
Reflections collected	14624	
Independent reflections	4248 (R(int) = 0.0190)	
Observed reflections	3404 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.38 and 0.73	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	4248 / 0 / 272	
Goodness-of-fit on F^2	1.06	
Final R indices (I>2sigma(I))	R1 = 0.047, wR2 = 0.116	
Largest diff. peak and hole	0.48 and -0.21 $eÅ^{-3}$	

5 Computational Investigation

5.1 Computational Details

All quantum chemical calculations were performed using Orca 5.0.1.[6,7] The structures were optimized using the B3LYP/G functional with the def2-TZVP basis set, as commonly used to enable comparison of the fundamental gap between different publications.[8–11] The structures were fully optimized and did not show any imaginary frequencies within the used level of theory.

5.2 Overview of the Computed Molecules

Table S6. Energies of all computed structures.

	E_{SCF} [Eh]	H [Eh]	G [Eh]	E_{HOMO} [eV]	E_{LUMO} [eV]	$E_{g(calc)}$ [eV]
2a	−2381.60685314	−2380.68959768	−2380.81354058	−5.4103	−1.6156	3.7947
2b	−2066.98608991	−2066.30375074	−2066.40673001	−5.4380	−1.6378	3.8002
2c	−2296.12685520	−2295.37455704	−2295.48804195	−5.3767	−1.5714	3.8053
2d	−2741.37607292	−2740.67721921	−2740.79577783	−5.6643	−1.8946	3.7697
2e	−3059.72953152	−3059.11942744	−3059.24225198	−5.7885	−1.9433	3.8452
2f	−2708.50819769	−2707.89348117	−2707.99570199	−5.4750	−1.7055	3.7695
2g	−2391.28803205	−2390.18290883	−2390.32574839	−5.4161	−1.5821	3.8340
2h	−1683.38487988	−1682.81468464	−1682.90491567	−5.4413	−1.6023	3.8390
2i	−1604.71530876	−1604.20335418	−1604.28740048	−5.5042	−1.6619	3.8423
8a	−1604.73960935	−1604.22778999	−1604.31196110	−5.6211	−1.7439	3.8772
8b	−2597.47893247	−2597.03954018	−2597.14304091	−5.9920	−2.0829	3.9091
8c	−1929.03969781	−1928.10538465	−1928.22994860	−5.5903	−1.6892	3.9011
8d	−1142.46564711	−1142.12435783	−1142.18927730	−5.6911	−1.7833	3.9078
BBICZ-3	−1110.37433770	−1110.00995064	−1110.07616654	−5.1230	−1.5103	3.6127

5.3 Coordinates of the Optimized Geometries

2a

C	-0.439237259470	1.287360545158	0.201970606138
C	0.957646222918	1.027710548978	0.165568462875
C	1.405298081054	-0.294835574902	0.182944932896
C	0.439013628092	-1.287882907716	0.202410676297
C	-0.957841749997	-1.028188172789	0.165830384643
C	-1.405535047347	0.294312070604	0.182641363499
N	0.633978580858	-2.670533182225	0.277617431719
C	-0.600270902844	-3.293846512876	0.297837691737
C	-1.610632493273	-2.320343347414	0.189688288060
C	-0.926238378442	-4.668865050706	0.472427403457
N	-0.634298511781	2.669991627904	0.276655210415
C	0.599893101006	3.293418941641	0.296807593421
C	1.610360356837	2.319963318819	0.188731218525
C	0.925593863308	4.668507808336	0.471484400271
C	2.326774729658	4.949508066198	0.519259514658
C	-0.016326540642	-5.740011467538	0.638612795878
C	-0.465734006352	-7.022508668450	0.843401949846
C	-1.843998822822	-7.297957591169	0.890591655871
C	-2.751334245435	-6.281392589918	0.732211589510
C	-2.327499675603	-4.949486775243	0.521241045783
N	3.295134567296	4.007102771322	0.354577501593
N	-3.295838582257	-4.006861661596	0.357082507731
C	2.968392844839	2.747229335271	0.168163933283
C	-2.968747160757	-2.747224282490	0.169930010530
C	0.015520034434	5.739309579545	0.638913558894
C	0.464736745433	7.021895050476	0.843650672686
C	1.842956397988	7.297771173930	0.889479032442

C	2.750433259496	6.281517378577	0.730013669434
C	4.107122009425	1.830702718799	-0.103868926897
C	-4.106933118269	-1.830123285905	-0.102639562383
C	5.270081043275	1.903952377919	0.666963702112
C	6.367798553457	1.112865092725	0.372388764554
C	6.371062214143	0.229234546952	-0.714811017266
C	5.210110975828	0.173225227267	-1.486081794977
C	4.097889805122	0.953121837114	-1.184731512207
C	-5.268863438983	-1.899281067413	0.670051225550
C	-6.365972767832	-1.107662708173	0.374374446649
C	-6.369783285271	-0.227862212988	-0.715950037702
C	-5.209721662106	-0.175781157072	-1.488813317794
C	-4.098019600127	-0.955953707847	-1.186277658708
C	1.929475294309	-3.271015224196	0.256349450743
C	2.443265106085	-3.766120248647	-0.939083702210
C	3.703070620455	-4.351512314742	-0.959944574796
C	4.455911422383	-4.429197446951	0.207202697042
C	3.948301275362	-3.916488902004	1.395895211252
C	2.685552298522	-3.336292466037	1.422930504074
C	-1.929924342089	3.270202038197	0.257627121829
C	-2.444369432936	3.768613474426	-0.936145422531
C	-3.704206670268	4.354019121091	-0.954639486995
C	-4.456493685864	4.428178511978	0.213088930577
C	-3.948293693003	3.912005918623	1.400037592046
C	-2.685425543020	3.331997279195	1.424783067421
C	7.618907557561	-0.611333370623	-1.019539944685
C	7.938010487624	-1.516499390997	0.188312355569
C	8.816310056381	0.326114885564	-1.283185918075
C	7.435254025889	-1.506831439630	-2.253470536578

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C	-8.814707530481	-0.325907312093	-1.284395228678
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H	-2.456906235910	0.535304426158	0.199523620812
H	1.045689950151	-5.556371577789	0.612576043866
H	0.249308942016	-7.825274798166	0.970680574677
H	-2.186269895124	-8.312599405362	1.050818645613
H	-3.817702799230	-6.462051062235	0.759138828874
H	-1.046458426906	5.555368066497	0.614061109201
H	-0.250421820627	7.824382485944	0.972001219821
H	2.185096266262	8.312462123004	1.049680978169
H	3.816771559494	6.462502783157	0.756081868940
H	5.307309286705	2.599701232242	1.494454818166
H	7.245316247811	1.196445504847	1.000895730570
H	5.156580232385	-0.478941362522	-2.345874839092
H	3.222493828325	0.891709898485	-1.818485389186
H	-5.305965673771	-2.592123625155	1.500011572591
H	-7.242694836189	-1.188018071734	1.004402616574
H	-5.156454635085	0.473494115937	-2.350826486849
H	-3.223183164329	-0.897285403103	-1.821084461885
H	1.847495605709	-3.701005607508	-1.840107355599
H	4.096728947767	-4.745611511368	-1.887994903306
H	5.437143352581	-4.885645327333	0.189506691461
H	4.532843598145	-3.971052444162	2.305087869329
H	2.276609768715	-2.941781958974	2.343769294687
H	-1.849089846530	3.706082936990	-1.837670599153
H	-4.098329240055	4.750823820273	-1.881336402765

H	-5.437795355127	4.884547391084	0.197202443423
H	-4.532441618682	3.963743994891	2.309648351972
H	-2.276045541362	2.934855706302	2.344294615431
H	7.108921095757	-2.196623431016	0.393505819526
H	8.829674783458	-2.115901810133	-0.011619730439
H	8.124129259944	-0.934749541955	1.091697406052
H	8.617967202958	0.979796949169	-2.134625139906
H	9.713685669514	-0.256923305604	-1.504027245287
H	9.032931044067	0.958076909591	-0.421385196455
H	6.613685586875	-2.214169983636	-2.125156094648
H	7.244653788532	-0.921677347985	-3.155032431965
H	8.345440804931	-2.085209352256	-2.423295029725
H	-7.107984700168	2.200350559418	0.387849569617
H	-8.828402289533	2.119289705718	-0.018486412914
H	-8.124224355068	0.940262419408	1.087701265166
H	-8.615833187606	-0.981389342705	-2.134290813220
H	-9.712222034671	0.256396137467	-1.506605987891
H	-9.030920933382	-0.955881830296	-0.421048447759
H	-6.611190252333	2.211981689802	-2.132060865347
H	-7.244384681997	0.918137361815	-3.158866477032
H	-8.343339862132	2.084340336673	-2.428677434397

2b

C	-2.053548147442	3.742664125289	-1.338864474517
C	-1.575666823156	5.029423568827	-1.556291604682
C	-1.887441716779	6.049994178606	-0.665293582977
C	-2.691488285588	5.778716877565	0.437045685253
C	-3.183108447914	4.496833127976	0.644462160704
C	3.216972097078	-4.508031269596	0.620752102155

C	2.730655432458	-5.790865951358	0.407219520950
C	1.903715256754	-6.053812749757	-0.680176397983
C	1.565154352480	-5.024131866886	-1.550514252661
C	2.038559041005	-3.736820605806	-1.326920453392
C	2.866698371793	-3.462449953892	-0.236758452041
C	-2.860387846097	3.460737909861	-0.234735432825
C	-3.448545630011	2.107825285610	-0.034607344268
C	3.449898042746	-2.108145368812	-0.031708606797
N	-4.751350875428	2.079922596516	0.135039643225
N	4.752230355194	-2.077163163153	0.142493114527
C	-5.400075462228	0.887717824187	0.249986076278
C	-6.802263765541	0.929168565555	0.422263112900
C	-7.538601052120	-0.223858279612	0.523490645748
C	-6.898714592038	-1.474391111675	0.455735916103
C	-5.536749827595	-1.554229152560	0.291335865174
C	5.398797042404	-0.884372696937	0.258603813026
C	6.799436621699	-0.924328027632	0.443655958808
C	7.534549624404	0.229441069402	0.545119872904
C	6.894781225791	1.479358950766	0.464430865423
C	5.534070841661	1.557527645217	0.288849444953
C	4.746607613053	0.386111664960	0.184590477637
C	2.670211184038	-0.918033685982	-0.042333850532
C	3.331967889072	0.321819980760	0.039023150370
N	2.395181200333	1.337301228844	0.010198296589
C	-4.748469963277	-0.383661279139	0.186197761063
C	-2.670944079776	0.916837233673	-0.043444164678
C	-3.333364361744	-0.321923343040	0.045612655517
N	-2.396910231464	-1.338021618950	0.024305095148
C	-0.099556402434	1.431872899748	-0.060267710974

C	-1.250298137335	0.641719375737	-0.070896017598
C	-1.119902168239	-0.772973288261	-0.039608442323
C	0.098080580722	-1.433580688082	-0.048568404123
C	1.249141215821	-0.643538825687	-0.068294695148
C	1.118466844377	0.771291552589	-0.047283952439
C	2.606872552565	2.749551848621	0.056025678859
C	2.531311679812	3.421342439988	1.272455966376
C	2.719384459812	4.797514794151	1.314018764368
C	2.978650042761	5.501954062953	0.143454029106
C	3.042670146411	4.829604047627	-1.072261760433
C	2.850888659425	3.453988800223	-1.119265697877
C	-2.610497177617	-2.750078138851	0.067835945285
C	-2.563205180236	-3.421301398847	1.285983305506
C	-2.756510482810	-4.796978672477	1.324676619959
C	-2.991764921945	-5.502046226266	0.149462994894
C	-3.026014215170	-4.830515537219	-1.067875345119
C	-2.829739438913	-3.455430732725	-1.111727564725
H	-1.814789493757	2.954949028458	-2.041985002866
H	-0.963430273416	5.235070826577	-2.425336802210
H	-1.512356006859	7.051821851110	-0.832431325948
H	-2.943123250017	6.569745966361	1.132434232752
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H	3.882477435781	-4.304772893934	1.448923299120
H	3.004062305636	-6.588988612180	1.086118424269
H	1.531702420264	-7.056018541472	-0.852009508261
C	-0.439237259470	1.287360545158	0.201970606138
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H	1.779336192338	-2.942525207895	-2.015141829198
H	-7.266397531749	1.905530204290	0.463782937901

H	-8.612449010601	-0.174041161508	0.652531658371
H	-7.481895392267	-2.383108699269	0.533667123533
H	-5.070869018819	-2.525501881665	0.244690950608
H	7.263302063785	-1.900362549302	0.494968184348
H	8.607200722356	0.180672712603	0.684148380590
H	7.476540794978	2.389020307282	0.541458352190
H	5.068559311323	2.528423401777	0.233657957548
H	-0.150481694709	2.509359818148	-0.045210071293
H	0.148988637511	-2.510857856832	-0.024054156852
H	2.332772074260	2.861335265987	2.176770874554
H	2.663851020352	5.318370275397	2.261058970348
H	3.126376886738	6.573641304861	0.177857603447
H	3.239807584671	5.375676103738	-1.985748002880
H	2.899233760356	2.918888513393	-2.058650904897
H	-2.383679021776	-2.861059261838	2.194178718247
H	-2.723774015657	-5.316973333657	2.273269084275
H	-3.143921470657	-6.573161932224	0.181786308294
H	-3.203955436299	-5.376693403501	-1.985229089181
H	-2.855056585712	-2.921456475018	-2.052634544255

2c

C	-5.538872059115	-0.709498331799	0.784866567400
C	-6.435301603168	0.326261919405	0.606291098438
C	-6.278017931253	1.216664357562	-0.459881325808
C	-5.210495697560	1.049562815523	-1.339858252155
C	-4.305505572991	0.011589615892	-1.134807492647
C	4.198337652518	-0.005737277204	-1.316764687948
C	5.100243123861	-1.015745345100	-1.599359906220
C	6.214070256050	-1.212524485565	-0.779667805290

C	6.413146113984	-0.375049927586	0.317597882718
C	5.506961799973	0.647150585739	0.577077817825
C	-4.444951379828	-0.877833962467	-0.073516904834
C	4.382040355031	0.844520091750	-0.220571834013
C	4.053946341943	5.487680105982	0.621406370906
C	3.395572187993	6.678671601511	0.794693500304
C	1.990190690159	6.715718316902	0.760947351868
C	1.266485810915	5.566595244146	0.550266118904
C	-3.532868622068	-2.037561385667	0.099383481573
C	3.479091283840	1.996354554102	0.035760036187
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C	-3.382149165940	-4.338055496660	0.368963240849
C	-4.081591826890	-5.551402489430	0.560452551679
C	-3.418387730215	-6.750966720432	0.619336682431
C	-2.018720003613	-6.787833466892	0.486581708785
C	-1.304078975077	-5.627797107612	0.306713127010
C	3.344321857717	4.284413277989	0.404657224129
C	1.915507121278	4.323166870068	0.362948916345
C	2.059262585447	1.885339880066	0.049216610970
C	1.291287066856	3.057643209930	0.174861136180
N	-0.050977363110	2.724557223398	0.164691722550
C	-1.957510781916	-4.373883477251	0.249935974602
C	-2.113886637120	-1.923785712938	0.055445463263
C	-1.340737342687	-3.098726069127	0.109320724579
N	-0.001043350679	-2.762340501574	0.061098065436
C	-1.332092580343	0.581222897314	0.068694608797
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C	-3.393547843	-2.128714962	0.000119217

H	0.170229168	2.517804112	0.000393139
H	-0.170218226	-2.517816953	-0.000275310
H	-2.611817326	2.301520298	-0.000546647
H	4.927329663	-2.551577061	0.000060975
H	7.371500170	-2.557813794	0.000363148
H	8.632781661	-0.417397495	0.000341001
H	7.427266848	1.726269618	-0.000013387
H	5.336937089	2.999695139	-0.000183429
H	-4.927298277	2.551569604	0.000073708
H	-7.371503511	2.557820345	-0.000409111
H	-8.632775621	0.417438226	-0.000480883
H	-7.427274482	-1.726261065	-0.000095533
H	-5.336934759	-2.999700703	0.000109357
H	2.611866171	-2.301514800	-0.000199798
H	2.880044349	3.082247366	-0.000066807
H	-2.880055029	-3.082248698	0.000040869

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